NEWS 1 Web Page for STN Seminar Schedule - N. America NEWS 2 AUG 10 Time limit for inactive STN sessions doubles to 40 minutes

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NEWS 4 AUG 24 ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced

NEWS 5 AUG 24 CA/Caplus enhanced with legal status information for U.S. patents

NEWS 6 SEP 09 50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY

NEWS 7 SEP 11 WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus

NEWS 8 OCT 21 Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded

NEWS 9 OCT 21 Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models

NEWS 10 OCT 27 Free display of legal status information in CA/CAplus, USPATFULL, and USPAT2 in the month of November.

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4, AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:17:16 ON 05 NOV 2009

=> file reg COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

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DICTIONARY FILE UPDATES: 3 NOV 2009 HIGHEST RN 1191028-08-6

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Uploading C:\Program Files\Stnexp\Oueries\10511564-butane-broad.str

STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

G1 O.N

SAMPLE SEARCH INITIATED 13:18:07 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -1209 TO ITERATE

100.0% PROCESSED 1209 ITERATIONS 15 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 22094 TO 26266 PROJECTED ANSWERS: 68 TO 532

L2 15 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 13:18:11 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 23159 TO ITERATE

100.0% PROCESSED 23159 ITERATIONS SEARCH TIME: 00.00.01

314 ANSWERS

1.3 314 SEA SSS FUL L1

Uploading C:\Program Files\Stnexp\Queries\10511564-hexane-broad.str

I.4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 14

G1 0, N

SAMPLE SEARCH INITIATED 13:22:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 306 TO ITERATE

100.0% PROCESSED 306 ITERATIONS

7 ANSWERS

66 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5071 TO 71

PROJECTED ITERATIONS: 5071 TO 7169
PROJECTED ANSWERS: 7 TO 298

L5 7 SEA SSS SAM L4

=> s 15 full

FULL SEARCH INITIATED 13:23:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5664 TO ITERATE

100.0% PROCESSED 5664 ITERATIONS

SEARCH TIME: 00.00.01

L6 66 SEA SSS FUL L4

=

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L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR

G1 O, N

Structure attributes must be viewed using STN Express query preparation.

-> s 17 full sss sub=4 4 IS NOT A VALID L# L-numbers must be in the range L1-L999. ENTER SUBSET L# OR (END):end SEARCH ENDED BY USER

=> s 17 full sss sub=16 FULL SUBSET SEARCH INITIATED 13:45:36 FILE 'REGISTRY'

FULL SUBSET SEARCH INITIATED 13:45:36 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 53 TO ITERATE

100.0% PROCESSED 53 ITERATIONS SEARCH TIME: 00.00.01

L8 0 SEA SUB=L6 SSS FUL L7

=> Uploading C:\Program Files\Stnexp\Queries\10511564-hexane-amine-acid.str

0 ANSWERS

L9 STRUCTURE UPLOADED

=> d 19 L9 HAS NO ANSWERS L9 STR

G1 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 19 full sss sub=16 FULL SUBSET SEARCH INITIATED 13:47:54 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED -4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS SEARCH TIME: 00.00.01

0 ANSWERS

0 SEA SUB=L6 SSS FUL L9 L10

Uploading C:\Program Files\Stnexp\Queries\10511564-hexane-amine-alk.str

L11 STRUCTURE UPLOADED

=> d 111 L11 HAS NO ANSWERS

L11 STR

Structure attributes must be viewed using STN Express query preparation.

=> s l11 full sss sub=16

SEARCH TIME: 00.00.01

FULL SUBSET SEARCH INITIATED 13:50:19 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS

0 ANSWERS

L12 0 SEA SUB=L6 SSS FUL L11

=>

G1 O, N

Uploading C:\Program Files\Stnexp\Queries\10511564-hexane-alk-alk.str

L13 STRUCTURE UPLOADED

=> d 113 L13 HAS NO ANSWERS

L13 STR

G1 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 113 full sss sub=16

FULL SUBSET SEARCH INITIATED 13:52:22 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 66 TO ITERATE

100.0% PROCESSED

66 ITERATIONS

16 ANSWERS

SEARCH TIME: 00.00.01

16 SEA SUB=L6 SSS FUL L13

L14

Uploading C:\Program Files\Stnexp\Queries\10511564-butane-alk-alk.str

L15 STRUCTURE UPLOADED

=> d 115

L15 HAS NO ANSWERS

L15 STR

G1 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 115 full sss sub=13

FULL SUBSET SEARCH INITIATED 13:54:14 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 131 TO ITERATE

100.0% PROCESSED 131 ITERATIONS

15 ANSWERS

SEARCH TIME: 00.00.01

L16 15 SEA SUB=L3 SSS FUL L15

=>

Uploading C:\Program Files\Stnexp\Queries\10511564-butane-amine-alk.str

L17 STRUCTURE UPLOADED

=> d 117 L17 HAS NO ANSWERS L17 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 117 full sss sub=13

FULL SUBSET SEARCH INITIATED 13:55:59 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 158 TO ITERATE

100.0% PROCESSED 158 ITERATIONS SEARCH TIME: 00.00.01 8 ANSWERS

L18 8 SEA SUB=L3 SSS FUL L17

G1 O.N

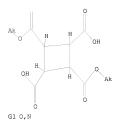
=> Uploading C:\Program Files\Stnexp\Queries\10511564-butane-acid-alk.str

L19 STRUCTURE UPLOADED

=> d 119

L19 HAS NO ANSWERS

L19 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 119 full sss sub=13

FULL SUBSET SEARCH INITIATED 13:57:32 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 93 TO ITERATE

100.0% PROCESSED 93 ITERATIONS 6 ANSWERS SEARCH TIME: 00.00.01

L20 6 SEA SUB=L3 SSS FUL L19

=> file caplus

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 SINCE FILE
 TOTAL

 FULL ESTIMATED COST
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 711.18

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FILE COVERS 1907 - 5 Nov 2009 VOL 151 ISS 19
FILE LAST UPDATED: 4 Nov 2009 (20091104/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

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=> s 120 or 118 or 116 or 114 12 L20 5 L18 59 L16 13 L14

L21 84 L20 OR L18 OR L16 OR L14

=> s 121 not py > 2003 8004419 PY > 2003 L22 72 L21 NOT PY > 2003

=> d 122 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 72 ANSWERS - CONTINUE? Y/(N):y

L22 ANSWER 1 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:196443 CAPLUS

DOCUMENT NUMBER: 138:221974

TITLE: Cyclobutanetetracarboxylic acid (meth)acrylate

derivatives and their manufacture INVENTOR(S): Suzuki, Hideo

INVENTOR(S): Suzuki, Hideo
PATENT ASSIGNEE(S): Nissan Chemical

PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------|------|----------|-----------------|----------|
| | | | | |
| JP 2003073338 | A | 20030312 | JP 2001-261039 | 20010830 |
| RIORITY APPLN. INFO.: | | | JP 2001-261039 | 20010830 |
| | | | | |

AB Title compds. I [R4-R7 = OH, (OC2H4)n02CCR1:CR2R3; R4 = R5 = R6 = R7 ± OH; R1 = H, Cl-4 alkyl; R2, R3 = H, Cl-10 alkyl; n = l-3] are manufactured by reaction of cyclobutanetetracroboxylic acid dianhydride (II) with R1R3C:CR1CO2(C2H4O)nH (R1-R3, n = same as I). I are useful as radically polymerizable or UV-curable monomers for transparent acrylic polymers (no data). Thus, II was esterified with 2-methacryloylethanol in p-methoxyphenol at 100° for 18 h to give 21.2% I (R4-R7 = OC2H4O2CCMe:CR12).

IT 500711-77-3P

RL: IMF (Industrial manufacture); PREP (Preparation)

(manufacture of cyclobutanetetracarboxylic acid (meth)acrylate derivs.)

RN 500711-77-3 CAPLUS

CN

1,2,3,4-Cvclobutanetetracarboxvlic acid, 1,2,3,4-tetrakis[2-[(2-methyl-1-oxo-2-propen-1-v1)oxy]ethyl] ester (CA INDEX NAME)

L22 ANSWER 2 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2002:592321 CAPLUS

DOCUMENT NUMBER: 137:161308

TITLE:

Dry silver heat-developable photographic film containing carbohydrazide reductant with improved mechanical strength

INVENTOR(S): Kato, Kazunobu

Fuji Photo Film Co., Ltd., Japan PATENT ASSIGNEE(S): SOURCE: Jpn. Kokai Tokkyo Koho, 55 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE JP 2002221768 20020809 JP 2001-17595 20010125 JP 2001-17595 PRIORITY APPLN. INFO.: 20010125 OTHER SOURCE(S): MARPAT 137:161308

The photog. film comprises, on a support, a photothermog. material containing AB an organic Ag salt, a hydrophobic organic binder, and a reducing agent (I) (A)kB

[k ≥2; Z is linked with B; B = connection group having k valance; B may be a polymer; Z = carbamoyl, acyl, sulfamoyl, alkoxycarbonyl, aryloxycarbonyl; Q = residue required to form an unsatd. ring with C]. The reducing agent crosslinks with the binder and hardens the film at the heat-developed region, so that the film shows high mech. strength after heat development.

445278-89-7

RL: TEM (Technical or engineered material use); USES (Uses) (dry silver heat-developable photog. film containing carbohydrazide reductant)

RM 445278-89-7 CAPLUS CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetrakis[2-[[[2-(2,5,6-trichloro-4-pyrimidinyl)hydrazinyl]carbonyl]amino]ethyl] ester (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

$$\begin{array}{c} \mathsf{C1} \\ \mathsf{N} \\ \mathsf{C} \\ \mathsf{1} \\ \mathsf{N} \\ \mathsf{N} \\ \mathsf{C} \\ \mathsf{1} \\ \mathsf{C} \\ \mathsf{1} \\ \mathsf{C} \\ \mathsf{1} \\ \mathsf{C} \\ \mathsf{1} \\ \mathsf{C} \\$$

PAGE 2-B

L22 ANSWER 3 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:489385 CAPLUS

DOCUMENT NUMBER: 135:77662

TITLE: Preparation of alicyclic epoxy ester for cured resin INVENTOR(S): Shimoda, Teruyoshi; Date, Hideki; Takahashi, Yasushi;

Hatanaka, Kohei

PATENT ASSIGNEE(S): Asahi Kasei K. K., Japan; Asahi Kasei Epoxy Co., Ltd. SOURCE: PCT Int. Appl., 226 pp.

PCT Int. Appl., 226 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PA | TENT | NO. | | | KIN | D | DATE | | | APPL | ICAT | ION | NO. | | D | ATE | |
|---------|-------|------|------|-----|-----|-----|------|------|-----|------|------|------|-----|-----|-----|-------|-----|
| WC | 2001 | | | | A1 | | 2001 | 0705 | | WO 2 | 000- | JP93 | 52 | | 2 | 0001 | 227 |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BY, | BZ, | CA, | CH, | CN, |
| | | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EE, | ES, | FI, | GB, | GD, | GE, | GH, | GM, | HR, |
| | | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KZ, | LC, | LK, | LR, | LS, | LT, |
| | | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NO, | NZ, | PL, | PT, | RO, | RU, |
| | | SD, | SE, | SG, | SI, | SK, | SL, | TJ, | TM, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VN, |
| | | YU, | ZA, | ZW | | | | | | | | | | | | | |
| | RW: | GH, | GM, | KE, | LS, | MW, | MZ, | SD, | SL, | SZ, | TZ, | UG, | ZW, | AT, | BE, | CH, | CY, |
| | | DE, | DK, | ES, | FI, | FR, | GB, | GR, | IE, | IT, | LU, | MC, | NL, | PT, | SE, | TR, | BF, |
| | | ΒJ, | CF, | CG, | CI, | CM, | GA, | GN, | GW, | ML, | MR, | NE, | SN, | TD, | TG | | |
| JE | 2001 | 1812 | 38 | | A | | 2001 | 0703 | | JP 1 | 999- | 3688 | 41 | | 1 | 9991: | 227 |
| JE | 2003 | 2862 | 76 | | A | | 2003 | 1010 | | JP 1 | 999- | 3693 | 80 | | 1 | 9991: | 227 |
| PRIORIT | Y APP | LN. | INFO | . : | | | | | | JP 1 | 999- | 3688 | 41 | - 2 | A 1 | 9991: | 227 |
| | | | | | | | | | | JP 1 | 999- | 3693 | 80 | | A 1 | 9991: | 227 |

OTHER SOURCE(S): MARPAT 135:77662

- AB Compound RXxYyZz is prepared for cured resin, wherein X is 2,3-epoxycyclohexyl ester or 2,3-epoxycyclopentyl ester, Y is epoxyalkyl ester and Z is alkyl ester, x + 1-20. yr=0-5, z=0-5, and x + y = 2-20. Thus,
 - 1,3,5-benzenetricarboxylic acid 2,3-epoxycyclohexyl ester prepared by transesterification of corresponding acid Me ester and
 - 3-hydroxycyclohexene followed by oxidation was mixed with curing agent at ratio 19.5/80.5 to give a product, showing good weather and water resistance.
- 14495-41-1
 - RL: RCT (Reactant); RACT (Reactant or reagent)
- (preparation of alicyclic epoxy ester for cured resin) RN 14495-41-1 CAPLUS
- CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



REFERENCE COUNT: 1.0 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN 1998:723573 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER: 129:343334 ORIGINAL REFERENCE NO.: 129:69929a,69932a

TITLE:

Preparation of cyclobutane-derivative inhibitors of squalene synthase and protein farnesyl transferase INVENTOR(S): Arendsen, David L.; Baker, William R.; Fakhoury,

Stephen A.; Fung, Anthony K. L.; Garvey, David S.; Mcclellan, William J.; O'connor, Stephen J.; Prasad, Rajnandan N.; Rockway, Todd W.; Rosenberg, Saul H.; Stein, Herman H.; Shen, Wang; Stout, David M.;

Sullivan, Gerard M.; Augeri, David J.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S., 45 pp., Cont.-in-part of U.S. Ser. No. 564,524,

abandoned. CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | KIND DATE | APPLICATION NO. | DATE |
|-----------------|-----------------|-------------------------|----------------|
| | | | |
| US 5831115 | A 19981103 | US 1996-626859 | 19960412 |
| CA 2218597 | A1 19961024 | CA 1996-2218597 | 19960418 |
| WO 9633159 | A1 19961024 | WO 1996-US5529 | 19960418 |
| W: CA, JP, MX | | | |
| RW: AT, BE, CH, | DE, DK, ES, FI, | FR, GB, GR, IE, IT, LU, | MC, NL, PT, SE |
| EP 821665 | A1 19980204 | EP 1996-912978 | 19960418 |
| EP 821665 | B1 20011004 | | |
| R: AT, BE, CH, | DE, DK, ES, FR, | GB, GR, IT, LI, LU, NL, | SE, PT, IE, FI |
| JP 11504017 | T 19990406 | JP 1996-531980 | 19960418 |
| EP 1090908 | A2 20010411 | EP 2000-124275 | 19960418 |

EP 1090908 A.3 20010516

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI AT 206390 Т AT 1996-912978 19960418 20011015 B2 19950421 PRIORITY APPLN. INFO .: US 1995-426553 US 1995-428357 B2 19950421 US 1995-564524 B2 19951129 US 1996-626859 A 19960412 EP 1996-912978 A3 19960418

WO 1996-US5529

W 19960418

MARPAT 129:343334 OTHER SOURCE(S):

AB The title compds (I; permitted substituent values are defined in the disclosure), useful for inhibiting protein farnesyl transferase and the farnesylation of the oncogene protein Ras, or for inhibiting de-novo squalene production resulting in the inhibition of cholesterol biosynthesis, are prepared Thus, $(1\alpha, 2\beta, 3\beta, 4\alpha)-1-[N-benzyl-N-$ [(4S,5S)-(4-hydroxy-5-methy1)-6-phenylhexy1]aminocarbony1]cyclobutane-2,3,4-tricarboxylic acid, prepared from propionaldehyde in 10 steps,

demonstrated a 92% inhibition of protein farnesyl transferase at 1µM. 184228-81-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclobutane-derivative inhibitors of squalene synthase and protein farnesyl transferase) 184228-81-7 CAPLUS

RN

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-bis(phenylmethyl) ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD OS.CITING REF COUNT: 3

(3 CITINGS)

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 3 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1998:235919 CAPLUS

DOCUMENT NUMBER: 128:270941 ORIGINAL REFERENCE NO.: 128:53641a,53644a

TITLE: Preparation and properties of high molecular weight polyamic ester having a cyclobutane moiety in the main

chain

AUTHOR(S): Hasegawa, Masaki; Miura, Hirohiko; Haga, Naoki;

Hayakawa, Akira; Saito, Kiyoshi CORPORATE SOURCE:

Department of Materials Science and Technology,

Faculty of Engineering, Toin University of Yokohama,

Yokohama, 225, Japan SOURCE:

High Performance Polymers (1998), 10(1), 11-21 CODEN: HPPOEX; ISSN: 0954-0083

Institute of Physics Publishing PUBLISHER:

DOCUMENT TYPE: Journal

LANGUAGE: English

Preparation and properties of the polyimide derived from cyclobutanetetracarboxylic dianhydride (CBDA) with diamines are

investigated, focusing on the interfacial polycondensation of cyclobutanetetracarboxylic acid di-Me ester dichloride (2a) with diamines. Di-Me ester was conveniently prepared from CBDA by refluxing in methanol solution Di-Me ester consists of two regio isomers; one is α-type (1a)

with centrosymmetry, the other is β -type (1b) with plane symmetry. Separation of the mixture into each of pure la and 1b was successfully

performed

by fractional crystallization The structure of the first fraction is la, which was determined by x-ray crystal anal. The second fraction was necessarily assigned to 1b. 1A was converted into 2a by the reaction with thionyl chloride. The interfacial polycondensation of 2a with diamines afforded a high mol. weight polyamic ester. Polyimide was obtained only by heating the polyamic ester to about $230-280\,^{\circ}\mathrm{C}$. The cyclobutane polyimide thus obtained was thermally stable up to 400°C, and less stable under hydrolysis than polypyromellitimide.

205655-16-9P, 1,2,3,4-Cyclobutanetetracarboxylic acid 1,3-dimethyl ester-2,4-dibutylamide

RL: SPN (Synthetic preparation); PREP (Preparation)

(model compound; preparation and properties of high mol. weight polyamic esters

having a cyclobutane moiety in the main chain)

205655-16-9 CAPLUS RN

CM

1,3-Cyclobutanedicarboxylic acid, 2,4-bis[(butylamino)carbonyl]-, dimethyl ester (9CI) (CA INDEX NAME)

2957-97-3P, 1,2,3,4-Cyclobutanetetracarboxylic acid 1,3-dimethyl ester 205655-11-4P, 1,2,3,4-Cyclobutanetetracarboxylic acid 1,3-dimethyl ester-2,4-dichloride-hexamethylenediamine copolymer, polyamic acid sru 205655-14-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid 1,3-dimethyl ester-2,4-dichloride-4,4'-oxydianilne copolymer, polyamic acid sru

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and properties of high mol. weight polyamic esters having a cyclobutane moiety in the main chain)

RN 2957-97-3 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

RN 205655-11-4 CAPLUS

CN Poly[iminocarbony1[2,4-bis(methoxycarbony1)-1,3cyclobutanediyl]carbonylimino-1,6-hexanediyl] (9CI) (CA INDEX NAME)

RN 205655-14-7 CAPLUS

CN Poly(oxy-1, 4-phenyleneiminocarbonyl(2, 4-bis(methoxycarbonyl)-1, 3cyclobutanediyl]carbonylimino-1,4-phenylene] (9CI) (CA INDEX NAME)

OS.CITING REF COUNT:

n THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD

(8 CITINGS) REFERENCE COUNT:

12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 6 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

1997:372557 CAPLUS ACCESSION NUMBER:

127:65594 DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 127:12539a,12542a

TITLE: Preparation of cyclobutanecarboxamide-derivative inhibitors of protein farnesyltransferase and squalene svnthase

INVENTOR(S): Stein, Herman H.; Baker, William R.; Fung, Anthony K. L.; Rosenberg, Saul H.; Rockway, Todd W.; Fakhoury,

Stephen A.; Garvey, David S.; Donner, B. Gregory; McClellan, William J.; O'Connor, Stephen J.; Prasad,

Rajnandan; Shen, Wang; Sullivan, Gerard M. Abbott Laboratories, USA

PATENT ASSIGNEE(S): Abbott Laboratories, U.S., 49 pp., Cont.-in

U.S., 49 pp., Cont.-in-part of U.S. Ser. No. 194,366,

abandoned. CODEN: USXXAM Patent

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. US 5631401 19970520 US 1995-378334 19950124 Α AU 9520444 A 19960801 AU 1995-20444 19950601 PRIORITY APPLN. INFO.: US 1994-194366 B2 19940209 US 1995-378334 A 19950126 OTHER SOURCE(S): MARPAT 127:65594

B² A² B¹ I

GI

AB The title compds. [I; Al, A2 = CON(R1)R2; R1 = H, (un)substituted alkyl, cycloalkyl, aryl, alkenyl, etc.; R2 = aryl, alkenyl alkynyl, (un)substituted alkyl, etc.; NR1R2 = (un)substituted heterocyclyl; B1, B2 = CO2R7; R7 = H, carboxy-protecting group), useful for inhibiting protein farnesyltransferase and de novo squalene production resulting in the inhibition of cholesterol biosynthesis, are prepared Thus, (10, 2B, 3B, 40; -1-(N-propy)-N-(4-phenoxybenzyl)aminocarbonyl]-3-[N-benzyl-N-(4-phenoxybenzyl)aminocarbonyl]-3-[N-benzyl-N-(4-phenoxybenzyl)aminocarbonyll-ylloyloyth age-2 4-dicarboxylic acid, prepared by

phenoxybenzyl)aminocarbonyl]cyclobutane-2,4-dicarboxylic acid, prepared by the amidation of 1,2,3,4-cyclobutanetetracarboxylic acid dianhydride with N-propyl-4-phenoxybenzyl amine and N-benzyl-4-phenoxybenzyl amine, demonstrated a 94% inhibition of protein farnesyltransferase at 1 uM.

IT 171348-95-1P 171349-43-2P 191284-55-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyclobutanecarboxamide-derivative inhibitors of protein farnesyltransferase and squalene synthase)

RN 171348-95-1 CAPLUS

1,3-Cyclobutanedicarboxylic acid, 2,4-bis[[methyl[(4-phenoxyphenyl)methyl]amino]carbonyl]-, dimethyl ester, (1α,2α,3β,4β)- (9CI) (CA INDEX NAME)

RN 171349-43-2 CAPLUS

CN 1,3-Cyclobutanedicarboxylic acid, 2,4-bis[[[(4-phenoxyphenyl]methyl]ghenylmethyl]amino[carbonyl]-, dimethyl ester, [(a,2,a,β,4β)- (9C1) (CA INDEX NAME)

Relative stereochemistry.

RN 191284-55-6 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-bis[(4-phenoxyphenyl)methyl] ester, (1 α ,2 β ,3 β ,4 α)- (CA INDEX NAME)

Relative stereochemistry.

IT 171349-59-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclobutanecarboxamide-derivative inhibitors of protein farnesyltransferase and squalene synthase)

RN 171349-59-0 CAPLUS

CN 1,3-Cyclobutanedicarboxylic acid, 2,4-bis[[[(4-phenoxyphenyl)methyl]propylamino]carbonyl]-, dimethyl ester, (1a,2a,3B,4B)- (9CI) (CA INDEX NAME)

OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN 1997:41540 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

126:59749

ORIGINAL REFERENCE NO.: 126:11733a,11736a

TITLE: Preparation of cyclobutane-derivative inhibitors of

squalene synthase and protein farnesyl transferase Arendsen, David L.; Baker, William R.; Fakhoury, INVENTOR(S): Stephen A.; Fung, K. L. Anthony; Garvey, David S.; McClellan, William J.; O'Connor, Stephen J.; Prasad,

Rajnandan N.; Rockway, Todd W.; et al. PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: PCT Int. Appl., 133 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----------------------------------|---------|-------------|-------------------|--------------------|
| | A1 | 19961024 | WO 1996-US5529 | 19960418 |
| W: CA, JP, MX
RW: AT, BE, CH, | DE, DK, | ES, FI, FR | , GB, GR, IE, IT, | LU, MC, NL, PT, SE |
| US 5831115 | A | 19981103 | US 1996-626859 | 19960412 |
| EP 821665 | A1 | 19980204 | EP 1996-912978 | 19960418 |
| EP 821665 | B1 | 20011004 | | |
| R: AT, BE, CH, | DE, DK, | ES, FR, GB. | , GR, IT, LI, LU, | NL, SE, PT, IE, FI |
| JP 11504017 | T. | 19990406 | JP 1996-531980 | 19960418 |
| AT 206390 | | | AT 1996-912978 | |
| PRIORITY APPLN. INFO.: | | | US 1995-426553 | |
| | | | US 1995-428357 | A 19950421 |
| | | | US 1995-564524 | A 19951129 |
| | | | US 1996-626859 | |
| | | | WO 1996-US5529 | |
| OTHER SOURCE(S): | MARPAT | 126:59749 | 10 1990 000029 | W 15500410 |

- AB The title compds (I, permitted substituent values are defined in the disclosure), useful for inhibiting protein farnesyl transferase and the farnesylation of the oncogene protein Ras, or for inhibiting de-novo squalene production resulting in the inhibition of cholesterol biosynthesis, are prepared Thus, (Ia, 2B, 3B, 4a)-IN-Denzyl-N-[(4S,5S)-(4-hydroxy-5-methyl)-6-phenylhexyl]mminocarbonyl]cyclobutane-2,3,4-tricarboxylic acid, prepared from propionaldehyde in 10 steps,
- demonstrated a 92% inhibition of protein farnesyl transferase at 1µM. 184228-81-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclobutane-derivative inhibitors of squalene synthase and protein farnesyl transferase)

RN 184228-81-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-bis(phenylmethyl) ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD

(3 CITINGS)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 8 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:978682 CAPLUS

DOCUMENT NUMBER: 124:29303

ORIGINAL REFERENCE NO.: 124:5623a,5626a

TITLE: Cyclobutane derivatives and their use as inhibitors of protein farnesyltransferase and squalene synthase
INVENTOR(S): Stein, Herman H.; Baker, William R.; Fung, Anthony K.
L.; Rosenberg, Saul H.; Rockway, Todd W.; Fakhoury,

Stephen A.; Garvey, David S.; Donner, B. Gregory;

Mcclellan, William J.; et al.

PATENT ASSIGNEE(S): Abbott Laboratories, USA SOURCE: PCT Int. Appl., 170 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
WO 9521815 A1 19950817 WO 1995-US1360 19950201

W: CA, JP, MX
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
PRIORITY APPLN. INFO: US 1994-194366 A 19940209

OTHER SOURCE(S): MARPAT 124:29303

GI

AB The invention provides compds. I [A1, A2 = CONR1R2, (CH2) nNR1R2, NHCONRIR2, CO2R4; R1 = H, alkvl, arvl, aralkvl, etc.; R2 = arvl, aralkvl, alkenyl, etc.; R4 = aryl, aralkyl, etc.; B1, B2 = CH2OH, CH:NOH, WR5, CO2H and derivs., etc.; W = bond, alk(en)ylene, CONH, NHCONH; R5 = various (un) substituted heterocyclics, etc.] and their pharmaceutically acceptable salts. I inhibit protein farmesyltransferase and the farmesylation of the oncogene protein Ras, as well as de novo squalene production, resulting in the inhibition of cholesterol biosynthesis. For example, reaction of trans-1,2,3,4-cyclobutanetetracarboxylic acid dianhydride with 4-(PhO)C6H4CH2NHCH2Ph in THF gave, after chromatog. separation of isomers, title compound II in 32% yield. II gave 98% inhibition of rat brain protein farnesyltransferase in vitro at 10 μM. Over 100 synthetic examples are given, plus data for inhibition of the title enzymes in vitro by selected compds.

ΙI

ΙT 171349-59-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of cyclobutane derivs. as inhibitors of protein farnesyltransferase and squalene synthase) 171349-59-0 CAPLUS

RN CN

1,3-Cvclobutanedicarboxylic acid, 2,4-bis[[[(4phenoxyphenyl)methyl]propylamino]carbonyl]-, dimethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

171348-95-1P 171348-96-2P 171349-43-2P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of cyclobutane derivs. as inhibitors of protein farnesyltransferase and squalene synthase)

RN 171348-95-1 CAPLUS

CN

1,3-Cyclobutanedicarboxylic acid, 2,4-bis[[methyl](4-phenoxyphenyl)methyl]amino]carbonyl]-, dimethyl ester, (1α,2α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 171348-96-2 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl 2,4-bis[(4-phenoxyphenyl)methyl] ester, (1a,2a,3B,4B)- (CA INDEX NAME)

Relative stereochemistry.

RN 171349-43-2 CAPLUS

CN 1,3-Cyclobutanedicarboxylic acid, 2,4-bis[[[(4phenoxyphenyl)methyl] (phenylmethyl)amino]carbonyl]-, dimethyl ester, (1\alpha, 2\alpha, 3\beta, 4\beta)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD (9 CITINGS)

L22 ANSWER 9 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1989:74416 CAPLUS

DOCUMENT NUMBER: 110:74416

ORIGINAL REFERENCE NO .: 110:12283a,12284a

Three puzzles for organic laboratory TITLE:

Todd, David; Pickering, Miles AUTHOR(S):

Worcester Polytech. Inst., Worcester, MA, 01609, USA CORPORATE SOURCE: SOURCE: Journal of Chemical Education (1988), 65(12), 1100-2

CODEN: JCEDA8; ISSN: 0021-9584

DOCUMENT TYPE: Journal

LANGUAGE: English

Three puzzles are described for organic labs., each of which can be solved using m.p. alone, and each of which involves work at the 100-200-mg scale. The 1st puzzle involves determining the product of the Friedel-Crafts acylation of 2-chlorotoluene with AcCl, the 2nd puzzle involves the determination of the product of the nucleophilic substitution of 3,4-dichloronitrobenzene with Na methoxide, and the 3rd puzzle involves determining the isomer formed from

the

photodimerization of maleic anhydride.

1032-95-7

RL: MSC (Miscellaneous)

(m.p. determination of, laboratory experiment in)

RN 1032-95-7 CAPLUS CN

1.2.3.4-Cvclobutanetetracarboxvlic acid, tetramethyl ester. $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT:

11 RECORD (11 CITINGS)

L22 ANSWER 10 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1985:577814 CAPLUS DOCUMENT NUMBER: 103:177814

ORIGINAL REFERENCE NO.: 103:28599a,28602a

TITLE: The behavior of stereoisomeric ions in the gas phase.

> 2 - negative and positive chemical ionization of cyclohexanehexacarboxylic methyl esters

THERE ARE 11 CAPLUS RECORDS THAT CITE THIS

Audisio, Guido; Grassi, Maria; Traldi, Piero; Daolio, AUTHOR(S):

Sergio

CORPORATE SOURCE: Ist. Chim. Macromol., Milan, 20133, Italy SOURCE:

Organic Mass Spectrometry (1985), 20(5), 327-30

CODEN: ORMSBG; ISSN: 0030-493X

DOCUMENT TYPE: Journal

LANGUAGE: English

The pos. and neg. ion chemical ionization mass spectra of the title esters were studied. The rel. abundance of fragment ions at m/z 401 in the pos. ion spectra obtained for the esters studied is directly dependent on the trend of the different isomers to epimerize. A 3-step mechanism involves protonation, epimerization, and fragmentation.

77117-51-2 83238-59-9 83861-33-0

94054-00-9 94054-01-0 94054-02-1

RL: PRP (Properties)

(neg. and pos. chemical ionization mass spectra of)

RN 77117-51-2 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\alpha,4\alpha,5\alpha,6\alpha)$ – (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83238-59-9 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1 α , 2 α , 3 β , 4 α , 5 α , 6 β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83861-33-0 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\alpha,4\beta,5\alpha,6\beta)-$ (9CI) (CA INDEX NAME)

RN 94054-00-9 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1 α ,2 α ,3 α ,4 α ,5 α ,6 β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 94054-01-0 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\beta,4\alpha,5\beta,6\beta)$ – (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 94054-02-1 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\beta,3\alpha,4\beta,5\alpha,6\beta)$ – (9C1) (CA INDEX NAME)

DOCUMENT NUMBER: 103:87249

ORIGINAL REFERENCE NO.: 103:14013a,14016a

TITLE: Stereochemical study of

1,2,3,4,5,6-(hexamethoxycarbonyl)cyclohexanes

AUTHOR(S): Farina, Mario; Grassi, Maria; Di Silvestro, Giuseppe CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milan, I-20133.

Italy
SOURCE: Journal of the American Chemical Society (1985),

107(18), 5100-4

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 103:87249

AB The cis, epi, myo, muco, chiro, and scyllo stereoisomers of the title compound were prepared directly from bicyclooctene precursors or by

compound were prepared cirectly from Dicyclooctene precursors or by epimerization, their structure being ascertained by NMR anal. and by x-ray anal. The stereochem. pathway of alkaline epimerization was found to be cis \rightarrow epi dblarw. muco. dblarw. chiro.dblarw. myo.dblarw. scyllo. A seventh compound, detected by qas chromatog. after a long reaction time, was

tentatively identified as neo. The most abundant isomer in the equilibrium mixture at 25° is myo; however, if one considers the difference in symmetry, the order of stability in terms of conformational energy is scyllo > myo > chiro > muco. An interesting regioselective phenomenon was observed during ozonolysis of a bicyclocotene precursor and was attributed to the different stereochem, environment of the two unsatd, atoms involved in

the reaction. T 83238-59-9P 83861-33-0P 94054-00-9P

94054-01-0P 94054-02-1P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and NMR of)

RN 83238-59-9 CAPLUS CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1\alpha,2\alpha,3\beta,4\alpha,5\alpha,6\beta)- (9CI) (CA INDEX

Relative stereochemistry.

RN 83861-33-0 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\alpha,4\beta,5\alpha,6\beta)$ - (9CI) (CA INDEX NAME)

RN 94054-00-9 CAPLUS CN 1,2,3,4,5,6-Cvclohe

1 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1 α ,2 α ,3 α ,4 α ,5 α ,6 β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 94054-01-0 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\beta,4\alpha,5\beta,6\beta)-$ (9C1) (CA INDEX NAME)

Relative stereochemistry.

RN 94054-02-1 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\beta,3\alpha,4\beta,5\alpha,6\beta)$ - (9CI) (CA INDEX NAME)

IT 77117-51-2P

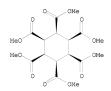
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, epimerization, and NMR of)

RN 77117-51-2 CAPLUS

1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1 α , 2 α , 3 α , 4 α , 5 α , 6 α) - (9CI) (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT:

(2 CITINGS)

L22 ANSWER 12 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1985:23948 CAPLUS

2

DOCUMENT NUMBER: 102:23948

ORIGINAL REFERENCE NO.: 102:3935a,3938a

TITLE: The behavior of stereoisomeric ions in the gas phase:

the case of cyclohexanehexacarboxylic methyl esters
AUTHOR(S): Audisio, Guido; Grassi, Maria; Daolio, Sergio; Traldi,

THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

Pietro

CORPORATE SOURCE: Ist. Chim. Macromol., CNR, Milan, 20133, Italy SOURCE: Organic Mass Spectrometry (1984), 19(5), 221-6

CODEN: ORMSBG; ISSN: 0030-493X

CODEN: ORMSBG; ISSN: 0030-493

DOCUMENT TYPE: Journal LANGUAGE: English

AB Not only strong differences in relative abundances of product ions, but also different fragmentation paths are observed in the electron impact mass spectroscopy of 6 stereoisomeric cyclohexanehexacarboxylic Me esters. This unusual behavior was studied using different ionization methods, B/E and B2/E linked scans, exact mass measurements, D labeling expts., and collisionally activated decomposition spectrometry. A close analogy between the isomerization observed under acidic conditions in condensed phase and that observed under chemical ionization (CH4) conditions is underlined.

IT 77117-51-2 83238-59-9 83861-33-0 94054-00-9 94054-01-0 94054-02-1 RL: PRP (Properties)

(mass spectrum of, electron-impact)

RN 77117-51-2 CAPLUS

1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\alpha,4\alpha,5\alpha,6\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83238-59-9 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1a,2a,3\beta,4a,5a,6\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 83861-33-0 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\alpha,4\beta,5\alpha,6\beta)$ – (9CI) (CA INDEX NAME)

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1 α , 2 α , 3 α , 4 α , 5 α , 6 β) - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 94054-01-0 CAPLUS $(D_1,2,3,4,5,6-C_2\text{Colohexanehexacarboxylic acid, hexamethyl ester,}\\ (1\alpha,2\alpha,3\beta,4\alpha,5\beta,6\beta)- (9CI) (CA INDEX NAME)$

Relative stereochemistry.

- RN 94054-02-1 CAPLUS
- CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, (1 α ,2 β ,3 α ,4 β ,5 α ,6 β)- (9C1) (CA INDEX NAME)

ORIGINAL REFERENCE NO.: 99:29923a,29926a

TITLE: cis, trans, cis- and

trans, trans, trans-1, 2, 3, 4-Tetravinylcyclobutane preparation and some spectroscopic properties Gleiter, Rolf; Haider, Rudolf; Gubernator, Klaus;

Bischof, Peter

Org. Chem. Inst., Univ. Heidelberg, Heidelberg, CORPORATE SOURCE:

D-6900, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1983), 116(8), 2983-93

CODEN: CHBEAM; ISSN: 0009-2940 DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:194460

AUTHOR(S):

AR Photochem. cyclization of di-Me fumarate gave I, which with NaOMe gave II. These were converted by standard means into the tetrakis (bromoethyl) derivs., dehydrohalogenation of which gave III and IV, resp., the photoelectron spectra of which showed strong interaction between the vinyl groups and the ring, but little interaction between the vinyl groups.

3999-67-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydride reduction of)

RN 3999-67-5 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester,

 $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

1032-95-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, isomerization, and hydride reduction of)

1032-95-7 CAPLUS RN

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT:

AUTHOR(S):

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 14 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1982:627952 CAPLUS

1

DOCUMENT NUMBER: 97:227952
ORIGINAL REFERENCE NO.: 97:38019a,38022a

TITLE: Crystal structures of:

r-1,c-2,t-3,c-4,t-5,c-6hexamethoxycarbonylcyclohexane, C18H24O12,

r-1-ethoxycarbonyl,c-2,t-3,c-4,t-5,c-6pentamethoxycarbonylcyclohexane, C19H26012 Brueckner, S.; Malpezzi, L.; Grassi, M.

CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy
SOURCE: Crystal Structure Communications (1982), 11(3), 1043-8
CODEN: CSCMCS; ISSN: 0302-1742

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hexamethoxycarbonylcyclohexane is orthorhombic, space group Pbca, with a 15.236(3), b 14.935(3), and c 18.936(4) Å; d. (calculated) = 1.328 for Z = 8; final R = 0.049. (Ethoxycarbonyl)pentamethoxycarbonylcyclohexane is monoclinic, space group P21/c, with a 9.278(2), b 22.802(4), c 11.564(3) Å, and β 112.70(3)*, d. (calculated) = 1.35 for Z = 4; final R = 0.56. Atomic parameters are given. Substitution of a Me group with an Et group in the ester residue axially connected to the cyclohexane ring does not involve significantly different intramol. interactions. The most relevant difference concerns the orientation of the carbomethoxy group connected to the cyclohexane ring through the C(5)-C(0) bond.
 B3834-82-6 83861-33-0

RL: PRP (Properties)
(crystal structure of)

RN 83834-82-6 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, ethyl pentamethyl ester, $(1\alpha,2\alpha,3\beta,4\alpha,5\beta,6\alpha)$ - (9CI) (CA INDEX NAME)

RN 83861-33-0 CAPLUS

1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha, 2\alpha, 3\alpha, 4\beta, 5\alpha, 6\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 15 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1982:561924 CAPLUS

DOCUMENT NUMBER: 97:161924

ORIGINAL REFERENCE NO.: 97:26997a,27000a TITLE: Ring inversion of

muco-1,2,3,4,5,6-hexakis(methoxycarbonyl)cyclohexane AUTHOR(S): Gatti, Giuseppe; Grassi, Maria; Di Silvestro, Giuseppe CORPORATE SOURCE: Ist. Chim. Macromol., Milan, I-20133, Italy

SOURCE: Journal of Chemical Research, Synopses (1982), (7),

CODEN: JRPSDC; ISSN: 0308-2342 DOCUMENT TYPE: Journal

LANGUAGE: English GI

AR

ester (II) with NaOMe in refluxing MeOH and by sequential ozonolysis, oxidation, and esterification of 5,7-exo-6,8-endotetrakis(methoxycarbonyl)bicyclo[2.2.2]oct-2-ene. 13C NMR study of I at -64 to +20° gave activation parameters ΔH^* = 11.79, $\Delta G^*(25^\circ)$ = 12.14 kcal/mol and ΔS^* = -1.2 cal/K/mol for ring inversion. The free-energy barrier to activation is considerably lower than for II (16.7 kcal/mol), owing to a decrease in the energy of

The title compound (I) was prepared by epimerization of the corresponding cis

the transition state due to smaller nonbonded interactions between substituents.

77117-51-2

RL: RCT (Reactant); RACT (Reactant or reagent) (epimerization of)

77117-51-2 CAPLUS RN

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha, 2\alpha, 3\alpha, 4\alpha, 5\alpha, 6\alpha)$ - (9CI) (CA INDEX

NAME)

Relative stereochemistry.

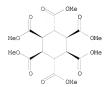
IT 83238-59-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and conformational inversion of, potential barrier to)

RN 83238-59-9 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\beta,4\alpha,5\alpha,6\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.



L22 ANSWER 16 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1982:526711 CAPLUS DOCUMENT NUMBER: 97:126711

ORIGINAL REFERENCE NO.: 97:21025a,21028a

TITLE: From cis,trans,cis-1,2,3,4-tetravinylcyclobutane to

cyclododecatetraene - two consecutive Cope

rearrangements

AUTHOR(S): Gubernator, Klaus; Gleiter, Rolf

CORPORATE SOURCE: Org.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.

SOURCE: Angewandte Chemie (1982), 94(9), 710-11

CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 97:126711

CT.

$$\begin{array}{c} \text{CH}_2 = \text{CH} \\ \text{CH}_2 = \text{CH} \\ \text{CH} = \text{CH}_2 \\ \text$$

I was prepared in a multistep synthesis from trans-MeO2CCH:CHCO2Me. I at 120° isomerizes almost quant. to a 63:23:14 II (and its cis-trans isomer)-III-IV mixture; the product ratio was temperature and medium independent.

VI

CH = CH2

CH=CH2

The reaction involves the Cope rearrangement of I to the common intermediate V via VI; V is unstable at these temps. and undergoes a second Cope rearrangement to give II or a 1,3-H shift to give III and IV. The products and I were characterized by 13C and 1H NMR.

1032-95-7

RL: RCT (Reactant); RACT (Reactant or reagent) (hydride reduction of)

1032-95-7 CAPLUS RN

 $CH = CH_2$

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, CN $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

AUTHOR(S):

L22 ANSWER 17 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN 1982:405471 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 97:5471

ORIGINAL REFERENCE NO.: 97:1067a,1070a TITLE: Ring reversal of

cis-cyclohexane-1,2,3,4,5,6-hexacarboxylic acid and

its hexamethyl ester

Gatti, Giuseppe; Grassi, Maria; Di Silvestro, Giuseppe; Farina, Mario; Bruckner, Sergio Inst. Chim. Macromol., CNR, Milan, 1-20133, Italy CORPORATE SOURCE: SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1982), (3), 255-8

CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal.

LANGUAGE: English

NMR studies showed that the title compds. (I and II, resp.) exist in solution at room temperature as an equilibrium of slowly exchanging chair

conformations. The

activation parameters were determined from complete line-shape anal. of the 13C NMR spectra measured at different temps. A relatively high value (.apprx.17 kcal/mol) of the free energy of activation was found for both I and II. The energy barrier of the acid was calculated by mol. mechanics and the computer program MOLBD3. The value obtained (16 kcal/mol) is a slight

overest., by comparison with the observed value of 13-14.5 kcal/mol. ΤТ 77117-51-2 RL: PRP (Properties)

(conformational inversion of, NMR and theor. study of) 77117-51-2 CAPLUS

RN CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha, 2\alpha, 3\alpha, 4\alpha, 5\alpha, 6\alpha)$ - (9CI) (CA INDEX

NAME)

Relative stereochemistry.

L22 ANSWER 18 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1981:148672 CAPLUS DOCUMENT NUMBER: 94:148672

ORIGINAL REFERENCE NO.: 94:24177a,24180a TITLE: The structure of

1,2,3,4,5,6-cis-cyclohexanehexacarboxylic acid and its

hexamethyl ester

AUTHOR(S): Brueckner, Sergio; Giunchi, Luciana Malpezzi; Di Silvestro, Giuseppe; Grassi, Maria

CORPORATE SOURCE: Ist. Chim., Politec. Milano, Milan, 20133, Italy SOURCE: Acta Crystallographica, Section B: Structural

Crystallography and Crystal Chemistry (1981), B37(3), 586-90

CODEN: ACBCAR; ISSN: 0567-7408

DOCUMENT TYPE: Journal LANGUAGE: English

C12H12O12.3H2O is orthorhombic, space group P212121, with a 13.44(1), b 11.18(1), c 10.37(1) \mathring{A} ; Z = 4; final R = 0.055. C18H24012 is

orthorhombic, space group Pbca, with a 34.79(3), b 20.63(2), and c 11.58(1) Å; Z = 8 (2 mols./Z); final R = 0.059. A comparison is drawn

between observed geometries and data calculated for a model mol. by the use of the mol.-mechanics method.

77117-51-2

RL: PRP (Properties) (structure of)

RN 77117-51-2 CAPLUS

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, hexamethyl ester, $(1\alpha,2\alpha,3\alpha,4\alpha,5\alpha,6\alpha)-$ (9C1) (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 19 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1975:46236 CAPLUS

DOCUMENT NUMBER: 82:46236

ORIGINAL REFERENCE NO.: 82:7351a,7354a

TITLE: Fuel for gasoline engines, containing nonaromatic

cyclic carboxylic acid ester
INVENTOR(S): Nottes, Guenter; Nohe, Heinz

PATENT ASSIGNEE(S): BASF A.-G.

SOURCE: Ger., 4 pp.
CODEN: GWXXAW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PR.

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|--------------------|------|----------|-----------------|---|----------|
| DE 2304068 | B1 | 19740606 | DE 1973-2304068 | | 19730127 |
| DE 2304068 | C2 | 19750130 | | | |
| DE 2316535 | A1 | 19741024 | DE 1973-2316535 | | 19730403 |
| NL 7315694 | A | 19740521 | NL 1973-15694 | | 19731115 |
| CA 1019571 | A1 | 19771025 | CA 1973-185873 | | 19731115 |
| FR 2207180 | A1 | 19740614 | FR 1973-40906 | | 19731116 |
| SU 466666 | A3 | 19750405 | SU 1973-1970238 | | 19731116 |
| AT 7309660 | A | 19750615 | AT 1973-9660 | | 19731116 |
| AT 328600 | В | 19760325 | | | |
| SE 383161 | В | 19760301 | SE 1973-15568 | | 19731116 |
| IT 1001797 | В | 19760430 | IT 1973-31411 | | 19731116 |
| GB 1442143 | A | 19760707 | GB 1973-53221 | | 19731116 |
| BE 807489 | A1 | 19740520 | BE 1973-137895 | | 19731119 |
| JP 49081408 | A | 19740806 | JP 1973-129287 | | 19731119 |
| JP 51039963 | В | 19761030 | | | |
| RITY APPLN. INFO.: | | | DE 1972-2256690 | A | 19721118 |
| | | | DE 1973-2304068 | A | 19730127 |
| | | | DE 1973-2316535 | A | 19730403 |

Additives like tetrakis(2-ethylhexyl) bicyclooctenetetracarboxyate [53525-50-1] and hexakis(2-ethylhexyl) cyclohexanehexacarboxylate (I) [53602-55-4] prevent formation of deposits on carburetors and therefore decrease the amount of CO in the exhaust. Thus, in a 1-cylinder test motor, run for 50 hr with fuel containing 500 ppm I, no deposits formed, corresponding to a demerit value of 10 on a 0-10 scale, whereas fuel containing 1000 ppm dioctyl phthalater rated 1. In an idling Fiat 600 D motor,

run with fuel containing 100 ppm I, CO output had not increased after 100 hr, whereas CO output increased from 3.7-4.4 to 7.1% within 50 hr when the fuel contained no I.

53602-55-4 53667-52-0

RL: USES (Uses) (gasoline detergent)

RN 53602-55-4 CAPLUS

1,2,3,4,5,6-Cyclohexanehexacarboxylic acid,

1,2,3,4,5,6-hexakis(2-ethylhexyl) ester (CA INDEX NAME)

53667-52-0 CAPLUS RN

CN 1,2,3,4,5,6-Cyclohexanehexacarboxylic acid, 1,2,3,4,5,6-hexakis(1-methylpropyl) ester (CA INDEX NAME)

L22 ANSWER 20 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

77:100953

ORIGINAL REFERENCE NO .: TITLE:

1972:500953 CAPLUS 77:16639a,16642a

AUTHOR(S):

Photodehydrocyclizations in stilbenelike compounds. V. Photochemistry of 2,2'-distyrylbiphenyl

Laarhoven, W. H.; Cuppen, Th. J. H. M.

Dep. Org. Chem., R. C. Univ., Nijmegen, Neth. Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999)

(1972), (16), 2074-9 CODEN: JCPRB4; ISSN: 0300-922X

CORPORATE SOURCE: SOURCE:

DOCUMENT TYPE: Journal LANGUAGE: English

For diagram(s), see printed CA Issue.

Irradiation of 2,2'-distyrylbiphenyl (I) in hexane under N for .apprx.15 min AB gave the kinetically-controlled product trans, trans, trans-1,2,2a, 10b-tetrahydro-1,2-diphenylcyclobuta[1]phenanthrene (II) but irradiation, for 6 hr gave 4,5,9,10-tetrahydro-4,9-diphenylphrene (III). Irradiation of I under N in the presence of iodine gave (-phenylbenzo[c]chrysene (IV). I in an evacuated tube at 240-50° for 2 hr gave, cis, cis, cis-1, 2, 2a, 10b-tetrahydro-1, 2-diphenylcyclobuta [1]phenanthrene (V). On irradiation or heating II reverted to I but V decomposed to

cis-stilbene and phenanthrene. 3999-67-5P 31351-41-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 3999-67-5 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

31351-41-4 CAPLUS DM

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\alpha, 4\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

SOURCE:

L22 ANSWER 21 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1972:24393 CAPLUS

DOCUMENT NUMBER: 76:24393 ORIGINAL REFERENCE NO.: 76:3967a,3970a

TITLE: Photochemical cycloaddition reactions. II. Dimerization and cycloadduct formation of some

seven-membered carbocycles AUTHOR(S): Kopecky, J.; Shields, J. E. CORPORATE SOURCE:

Ustav Prum. Hyg., Prague, Czech.

Collection of Czechoslovak Chemical Communications (1971), 36(10), 3517-26

CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 76:24393

AB The photochem. behavior of 2,3,6,7-dibenzocycloheptatrien-1-one (I), 2,3,6,7-dibenzocycloheptatriene and 1-methylene-2,3,6,7-dibenzocycloheptatriene (II), individually and in the

presence of each other, was studied. Irradiation of solns of these substances gave anti cyclobutane dimers and adducts; reactions occurred exclusively at the endocyclic olefinic sites in I and II. This observed photospecificity is supported by MO calcus. of delocalization energies for the possible reactive sites in the monomers. The elucidation of structures, thermal decomposition, chemical interconversions, and

stereochemistry
of the photoproducts are described.

I 1032-95-7P 31351-41-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, (1α,2α,3β,4β)- (CA INDEX NAME)

Relative stereochemistry.

RN 31351-41-4 CAPLUS

CN

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\alpha,4\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 22 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1971:411703 CAPLUS DOCUMENT NUMBER: 75:11703

ORIGINAL REFERENCE NO.: 75:1873a,1876a

TITLE: Structure of a planar cyclobutane.

Cis,trans,cis-1,2,3,4-cyclobutanetetracarboxylic acid

AUTHOR(S): tetramethyl ester Margulis, Thomas N.

CORPORATE SOURCE: Dep. Chem., Univ. Massachusetts, Boston, MA, USA SOURCE: Journal of the American Chemical Society (1971),

93(9), 2193-5

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: English

AB A single-crystal x-ray diffraction study of the title compound shows the cyclobutane ring to be planar with C-C bond lengths of 1.572 ± 0.005 and 1.541 ± 0.004 Å. The crystals are triclinic, space group P,

with a = 8.939, b = 5.963, and c = 6.454 Å; α = 95.17, β = 81.43, γ = 78.74°; Z = 1 and calculated d. = 1.45. The structure

was refined to an R value of 0.035 for 833 independent reflections.

RL: PRP (Properties)
(crystal structure of)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L22 ANSWER 23 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1971:75813 CAPLUS

DOCUMENT NUMBER: 74:75813
ORIGINAL REFERENCE NO.: 74:12299a,12302a

TITLE: Photochemistry of α, β-unsaturated

γ-lactones. I. Structures of the photodimers

of 4-hydroxycrotonic acid γ -lactone

AUTHOR(S): Ohga, Kazuya; Matsuo, Taku

CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, Japan SOURCE: Bulletin of the Chemical Society of Japan (1970),

43(11), 3505-10

CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

The structures of the photodimers obtained from 4-hydroxycrotonic acid γ -lactone under several conditions were determined The products of irradns. in the solution were a pair of anti-dimers: one is a head-to-head cycloadduct (I) and the other a head-to-tail adduct (II). The

corresponding product in the solid state, on the other hand, was a head-to-head cycloadduct (III), in the syn form.

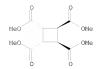
IT 1032-95-7P 31351-41-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 1032-95-7 CAPLUS

AB

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)



RN 31351-41-4 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\alpha, 4\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD 5 (5 CITINGS)

L22 ANSWER 24 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:487884 CAPLUS DOCUMENT NUMBER: 73:87884

ORIGINAL REFERENCE NO.: 73:14365a,14368a

TITLE: Effect of radiation on stable nucleic acid. 19.

Synthesis of the cis/syn- and cis/anti-dimeric uracils

AUTHOR(S): Richter, Peter; Fahr, Egon CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, Fed.

Rep. Ger.

SOURCE: Tetrahedron Letters (1970), (22), 1921-3

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB The cis/anti- and cis/syn-dimeric uracils (I) and (II), resp., were prepared Thus, refluxing III in MeOH gave IV (R = OH) and V (R = OH). IV (R = OH) was heated in CHC13 with PC15 to give IV (R = C1) which was treated with NaN3 in CHCl3 to give IV (R = N3). Refluxing IV (R = N3) in PhMe under N gave VI (R = NCO) which was converted to VI (R = NHCONH2) by NH3 in CHCl3. I (4%) and uracil were prepared by heating VI (R = NHCONH2) with 2N HCl at 65-70°. The ir spectrum of I was identical with that of the product of uv irradiation of uracil. II was similarly prepared from V (R =

OH). 28972-38-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 28972-38-5 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, cis-1,2,cis-1,3,cis-1,4- (8CI) (CA INDEX NAME)

OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 25 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: DOCUMENT NUMBER:

1970:132351 CAPLUS 72:132351

ORIGINAL REFERENCE NO.: 72:23687a,23690a

TITLE:

Preparation and properties of some 1,1'-diphenyl-syn, trans-truxane[9,10-diphenyl-syn, trans-4b, 4c, 9, 9z, 9b, 10-hexahydrocyclobuta[1, 2-a:4, 3-

a]diindene]derivatives

AUTHOR(S):

CORPORATE SOURCE: Univ. of Arkansas, Little Rock, AR, USA

Setliff, Frank L. SOURCE: Proceedings of the Arkansas Academy of Science (1969).

> 23, 177-82 CODEN: AKASAO; ISSN: 0097-4374

DOCUMENT TYPE: Journal.

LANGUAGE: English

exo,exo-1,1'-Dibromo-syn,trans-truxane (I) was treated with PhMgBr in the presence of CoC12 in ether-benzene to yield 51%

exo, exo-1,1'-diphenyl-syn, trans-truxane (II), m. 205-6°

(methylcyclohexane). II was also prepared (in 20% yield) by the alkylation of C6H6 with I in the presence of AlCl3 (12 hr at room temperature and 1 hr at 50°). Longer reaction times or higher temps, cause the

disappearance of II and give 30% exo, endo-1, 1'-diphenyl-syn, trans-truxane (III), m. 147-9°. II isomerizes to III (37% yield) with excess

AlC13 in C6H6 with gaseous HCl. The exo, exo isomer was assumed to be the more stable; two sequences are offered to explain the II → III

isomerization. Degradative ozonolysis of II and III in AcOH at room temperature, followed by esterification of the acid product with CH2N2 give cis, trans-1, 2, 3, 4-tetracarbomethoxy-cyclobutane.

1032-95-7P

CN

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 1032-95-7 CAPLUS

1,2,3,4-Cvclobutanetetracarboxvlic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

L22 ANSWER 26 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1970:42919 CAPLUS DOCUMENT NUMBER: 72:42919

ORIGINAL REFERENCE NO.: 72:7855a,7858a

Cyclobutanes, XXIV, Rearrangement of the TITLE .

tricyclo[4.2.0.02.5]octane system into the

tricyclo[4.2.0.02.4]octane system Avram, Margareta; Mateescu, Gheorghe D.; Dinulescu, AUTHOR(S):

Ilie G.; Nenitzescu, Costin D.

CORPORATE SOURCE: Org.-Chem. Inst., Akad. R.S.R., Bucharest, Rom.

SOURCE: Chemische Berichte (1969), 102(12), 4008-16

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

For diagram(s), see printed CA Issue. AB

Addition of Br to anti-tricyclo[4.2.0.02,5]octa-3,7-diene yielded two 3,4,7,8-tetrabromo-anti-tricyclo[4.2.0.02,5]octanes (I and II) which showed cis-trans isomerism of the Br atoms 7 and 8. I and II gave upon base treatment 3,7(or 3,8)-dibromo-anti-tricyclo[4.2.0.02,5]octa-3,7diene. I and II gave upon heating the corresponding

3,5,7,8-tetrabromo-anti-tricyclo[4.2.0.02,4]octanes (III and IV, resp.).

1032-95-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 1032-95-7 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT:

(1 CITINGS)

L22 ANSWER 27 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1969:469903 CAPLUS

DOCUMENT NUMBER: 71:69903

ORIGINAL REFERENCE NO.: 71:12881a,12884a TITLE:

Photolytic transformations of cis, cis-cyclodeca-3, 8-diene-1, 6-dione

Stankorb, Jerry W.; Conrow, Kenneth AUTHOR(S): CORPORATE SOURCE: Kansas State Univ., Manhattan, KS, USA SOURCE: Tetrahedron Letters (1969), (28), 2395-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

For diagram(s), see printed CA Issue.

Irradiation of cis, cis-cyclodeca-3, 8-diene-1, 6-dione (I) in Me2CO 2.5 hrs. gave 4 products including 60% tricyclic diketone (II, R = H2) (IIa). IIa refluxed in EtOH with BzH and a catalytic amount of piperidine yielded 85% tetrabenzylidene derivative (II, R = PhCH) (IIb), m. 211-12°. Ozonolysis of IIb, followed by oxidative work-up and esterification with

CH2N2 yielded 33% tetramethyl 1,2,3,4-cyclobutanetetracarboxylate (III),

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD

m. 147°. The tricyclo[4.4.0.02,7] isomer (IV) could only give the trans, trans, trans-tetracarboxylate. The tricyclic diketone (V) was converted to the dibenzylidene derivative (VI, R = O), m. 269°, in 87% vield, reduced by 1:2 LiAlH4-AlC13 to 3,8-dibenzylidenetricyclo[5,3,0,02,6]decane (VI, R = H) (VII), m. 123-4°, in 22% yield. Oxidation of VII with NaIO4-KMnO4 in aqueous dioxane gave 44.4% IIa. Baeyer-Villiger oxidation of the tricyclic diketone gave only 1 dilactone, m. 211-12°, presumably arising from IIa and not from the isomer IV which should produce 2 lactones. IIa was identical with the supposed cis, syn,cis-tricyclo[5.3.0.02,6]decane-4,9-dione of Shani (1968) by trans-ketalization with MeC(OMe)2Me and p-MeC6H4SO3H to give the reported diketal. IIa gave an oxime, m. 255-8°. IIa and a molar equivalent of N2H4.H2O gave a high yield of an azine (VIII), m. 295° (decomposition), v 3320, 1740, 1655 cm.-1, indicating residual CO groups and terminal NH2. VIII was accordingly formulated as a linear polymer with CO and hydrazone end groups. Upon electron impact or thermal decomposition retrocyclization in the 4-membered ring gives fragments (IX,X) of various sizes accounting for the mass spectrum, m/e 160, 242, 320, 402, 480, 562. Evidently I undergoes cis-trans isomerization either prior to, or concerted with, photocyclization. IIa is obtained from I even under conditions where no photosensitization may be expected. Under these conditions $n-\pi^*$ excitation and intersystem crossing to a triplet state is followed by intramol, energy transfer to one of the double bond π systems. Isomerization and cyclization may then ensue in this or subsequent excited states. 14495-41-1P

RN

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Photolytic transformations of cis, cis-cyclodeca-3, 8-diene-1, 6-dione) 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

L22 ANSWER 28 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1969:106459 CAPLUS DOCUMENT NUMBER:

70:106459

ORIGINAL REFERENCE NO.: 70:19879a,19882a TITLE:

Action of radiation on nucleic acid components. XVI. Synthesis of trans/syn- trans/anti-dimeric uracil

Richter, P.; Fahr, Egon AUTHOR(S):

CORPORATE SOURCE: Univ. Wuerzburg, Wuerzburg, Fed. Rep. Ger. SOURCE:

Angewandte Chemie, International Edition in English

(1969), 8(3), 208-9 CODEN: ACIEAY; ISSN: 0570-0833

DOCUMENT TYPE: Journal LANGUAGE: English

trans-1,2,3,4-Cyclobutanetetracarboxylic acid dianhydride is converted to trans-1, 2-bis(3-methylureido)-trans-3, 4-cyclobutanedi-carboxylic acid di-Me ester (I); the trans-1,3-trans-2,3-isomer (II) of I is prepared from a di-Me trans-1,3-cyclobutanedicarboxylate. I and II are heated with 2N HCl to give the title dimers.

ΙT 22555-07-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

22555-07-3 CAPLUS RN

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, CN cis-2,trans-3,trans-4- (8CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L22 ANSWER 29 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:28305 CAPLUS DOCUMENT NUMBER: 66:28305

ORIGINAL REFERENCE NO.: 66:5335a,5338a

TITLE:

Maleic anhydride-hexamethylbenzene mixtures in methylcyclohexane solution and in the solid state.

II. Photochemical and thermal reactions

AUTHOR(S): Raciszewski, Zbigniew

CORPORATE SOURCE: Union Carbide Corp., South Charleston, WV, USA

SOURCE: Journal of the Chemical Society [Section] B: Physical

Organic (1966), (12), 1147-55 CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. preceding abstract A methylcyclohexane solution of maleic anhydride and hexamethylbenzene was irradiated with uv light in the absence and in the presence of filters that confined absorption, either nearly or completely, to the maleic anhydride-hexamethylbenzene charge-transfer complex. In the latter case the reaction mixture also contained toluene in a 6- and 25-fold molar excess over hexamethylbenzene. Pentamethylbenzylsuccinic anhydride and resinous substances were isolated in all expts, but no adducts of toluene with maleic anhydride were found. Evidence was obtained for formation of CO2 during the irradiation. Uv irradiation of a mixture of maleic anhydride and hexamethylbenzene in the solid state produced 1,2,3,4-cyclobutanetetracarboxylic acid dianhydride (I). No adducts of hexamethylbenzene with maleic anhydride were detected. From a partly carbonized mixture obtained by heating equimolar quantities of maleic anhydride and hexamethylbenzene to 250° for 15.5 hrs. and followed by hydrolysis were isolated pentamethylbenzylsuccinic acid, 4,5,6,7-tetramethylindan-1,2-dicarboxylic acid, and resinous materials. Only 4,5,6,7-tetramethylindan-1,2-dicarboxylic acid and the resins were isolated in a similar experiment but with the heating time extended to 17 hrs. No detectable reaction occurred at 200° over a period of 14 hrs. Large contribution of the dative structure to the electronically excited complex (about 90%) resulted in the proton transfer within the complex to give a geminate pair of free radicals that combined yielding pentamethylbenzylsuccinic anhydride. The course of the photochem. reaction in the solid state reflected the absence of the charge-transfer complex and the limited mobility of the components of the solid matrix. Crystalline products obtained in the thermal reactions probably originated from the addition of the pentamethylbenzyl radical, formed by cleavage of the benzylic C-H bond in hexamethylbenzene, to maleic anhydride.

14495-41-1P

RN

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

14495-41-1 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA CN INDEX NAME)



L22 ANSWER 30 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:28280 CAPLUS DOCUMENT NUMBER: 66:28280

ORIGINAL REFERENCE NO.: 66:5327a,5330a

TITLE: Configuration analysis of cyclobutane by N.M.R.

spectroscopy

AUTHOR(S): Weitkamp, Horst; Korte, Friedhelm

CORPORATE SOURCE: Univ. Bonn, Bonn, Germany

SOURCE: Tetrahedron, Supplement (1966), No. 7, 75-87

CODEN: TETSAE; ISSN: 0563-2072 DOCUMENT TYPE:

Journal

LANGUAGE: German

AB A detailed analysis of 20 cyclobutanes is given. The magnetic shielding parameters are between $\tau = 6.2$ and 8.2 ppm. depending on the substituents. The effects of the substituents on the shift values for the ring protons were calculated The geminal and vicinal spin-spin coupling constant have the same size. The geminal coupling constant is opposite in sign to the vicinal ones, and, from theoretical considerations, assumed to be neg. The differences between the cis- and trans-vicinal coupling consts. are often very small, though the ratio Jcis/Jtrans is always larger than 1. The magnitudes are - 11 to -14 cycles/sec. for the geminal, +8 to +12 cycles/sec. for the cis-vicinal, and +8 to +10

cycles/sec. for the transvicinal coupling consts. 14495-41-1

RL: PRP (Properties)

(configuration and N.M.R. of)

14495-41-1 CAPLUS RN

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



L22 ANSWER 31 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:507417 CAPLUS DOCUMENT NUMBER:

65:107417

ORIGINAL REFERENCE NO.: 65:19967h,19968a-d

TITLE: Effect of radiation on nucleic acid components, VII.

Synthesis of uracil trans-dimers

AUTHOR(S): Doerhoefer, G.; Fahr, E. Univ. Wuerzburg, Germany

Tetrahedron Letters (1966), (37), 4511-16

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: German

For diagram(s), see printed CA Issue.

cf. CA 65, 949h. Tetra-Et trans-cyclobutane tetracarboxylate, prepared by photochem. dimerization of trans-HO2CCH:CHCO2H, saponified and treated with Ac20 gave the anhydride (I), m. 300°. I heated in NH4OH gave the amido-carboxylic acids (II, R = CONH2), C8H10N2O6, m. >300° (di-Me ester, m. >300°, prepared by methylation with CH2N2). The product was chromatog. unique but on submission to Hofmann degradation gave a very hygroscopic mixture of diaminocyclobutane dicarboxylic acids II (R = NH2) (III); tolylsulfonate m. 226-8°. II reacted with KCN gave the mixture (IV). IV was less thermally stable than the photochem, prepared cis-(5,5/6,6)dimeric uracil (V) and could not be recrystd. from H2O. Irradiation with shortwave uv light transformed IV into uracil. Paper chromatog. (7:3 PrOH-H2O) of IV and V gave the same Rf value but thin-layer chromatog, on silica gel (7:3 PrOH-H2O) gave Rf 0.50-0.53 for the photochem, prepared dimer V and Rf 0.60-0.63 for the synthetic dimer IV. Alkaline degradation 60 h. in 10 N aqueous NaOH at 50° reconverted IV to III, identified by the tolylsulfonate. The purely chemical synthesis of trans dimeric uracils demonstrated the presence of a cyclobutene system and showed to what extent the trans linkage of the pyrimidine rings in contrast to the cis dimerization by photochem. means, altered the properties of the dimer.

13375-98-9

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 13375-98-9 CAPLUS

CN 1,3-Cyclobutanedicarboxylic acid, 2,4-dicarbamoyl-, dimethyl ester, cis-1,2,trans-1,3,trans-1,4- (8CI) (CA INDEX NAME)

Relative stereochemistry.

91059-89-1P, 1,3-Cyclobutanedicarboxylic acid, 2,4-dicarbamoyl-, dimethvl ester

RL: PREP (Preparation) (preparation of)

RN 91059-89-1 CAPLUS

1,3-Cyclobutanedicarboxylic acid, 2,4-dicarbamoyl-, dimethyl ester (7CI) CN (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{N} & \mathsf{O} & \mathsf{O} \\ \mathsf{H}_2\mathsf{N} - \mathsf{C} & \mathsf{C} - \mathsf{OMe} \end{array}$$

L22 ANSWER 32 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:507416 CAPLUS DOCUMENT NUMBER: 65:107416

ORIGINAL REFERENCE NO.: 65:19967g-h

TITLE: Diazo compounds. XXV. Kinetic studies of the

photolysis and of the thermal decomposition of diazomethane in cyclohexane and cyclohexene AUTHOR(S): Mueller, Eugen; Renner, R.; Rundel, W.

CORPORATE SOURCE: Univ. Tuebingen, Germany

SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, Biochemie, Biophysik, Biologie (1966), 21(8), 751-5

CODEN: ZENBAX: ISSN: 0044-3174

DOCUMENT TYPE: Journal LANGUAGE: German

cf. CA 64, 19512e. The kinetics of the photolysis of diazomethane (I) in cyclohexane, mixts. of cyclohexane-cyclohexene (molar ratio 25:1), and cyclohexene are identical, indicating a similar mechanism, probably a

carben mechanism; the presence of O accelerates the photolysis of I in cyclohexane by a factor of 6. The thermal decompn, of I in the dark in cyclohexane is a 1st order reaction with a half life period of 74 hrs. at 25°.

13375-98-9

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 13375-98-9 CAPLUS

CN 1,3-Cyclobutanedicarboxylic acid, 2,4-dicarbamoyl-, dimethyl ester, cis-1,2,trans-1,3,trans-1,4- (8CI) (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 33 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1966:472656 CAPLUS

DOCUMENT NUMBER: 65:72656 ORIGINAL REFERENCE NO.: 65:13490a-d

TITLE: Photochemistry of crystalline dimethyl all-trans-hexatrienel,6-decarboxylate Lahav, M.; Schmidt, G. M. J.

AUTHOR(S): CORPORATE SOURCE: Weizmann Inst. Sci., Rehovoth, Israel SOURCE: Tetrahedron Letters (1966), (26), 2957-62 CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

LANGUAGE: English
GI For diagram(s), see printed CA Issue.

AB Di-Me all-trans-hexatriene-1,6-dicarb oxylate, I, m. 172° (alc.), irradiated under Pyrex glass 6 days in sunlight (A > 290 mu) and the mixed product chromatographed from a min. amount of CHCl3 on silica gel, eluted with C6H6 to remove I and again with 9:1 C6H6-CHCl3 gave 22% di-Me trans-1,3-bis[4-(1-carbomethoxy)buta-1-trans,3-trans-dienyl]cyclobutane-

trans-1,3-bis[4-(1-carbomethoxy) buta-1-trans,3-trans-dieny][cyclobutane-2,4-dicarboxylate (II), m. 139-40°. II submitted to ozonolysis in AcOH 2 hrs. and the mixture treated with 20% H2O2 gave trans-1,3-dicarbomethoxycyclobutane-trans-2,4-dicarboxylic acid, m. 179-80° (Me2CO). In the triclinic crystal structure of I, all mols. are likely to be parallel by analogy with the crystal structure of di-Me trans-trans-muconate. Since the unit cell does not have a 4-A. axis the only other sym. dimer to be expected from a topochemically controlled reaction is II. The formation of a cyclodimer from a crystalline hexatriene

derivative showed that this solid state reaction occurred with a min. amount of mol. motion since the trans configuration of the triene system was preserved and no other dimers or rearranged monomeric compds. were observed.

IT 2957-97-3 13160-90-2

(Derived from data in the 7th Collective Formula Index (1962-1966)) N 2957-97-3 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

RN 13160-90-2 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 22555-07-3 CAPLUS

 ${\tt CN} \hspace{0.5cm} 1,2,3,4-{\tt Cyclobutanetetracarboxylic\ acid,} \hspace{0.1cm} 1,3-{\tt dimethyl\ ester,}$

L22 ANSWER 34 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1966:472655 CAPLUS

DOCUMENT NUMBER: 65:72655

ORIGINAL REFERENCE NO.: 65:13489h,13490a

TITLE: Vapor phase photochemistry of 1,3-butadiene-1,1,4,4-d4 AUTHOR(S): Haler, I.; Srinivasan, R.

Watson Res. Center, Intern. Business Machines, CORPORATE SOURCE:

Yorktown Heights, NY SOURCE: Journal of the American Chemical Society (1966),

88(16), 3694-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: English

The mechanisms of the 3 primary processes in the vapor phase photolysis of 1,3-butadiene were investigated by the use of D labeling on the end C atoms. None of the processes proceeds by the obvious pathway exclusively.

Thus, ethylene and acetylene are formed not only by a 1,3 shift but also via an intermediate cyclobutene and a third path which gives C2H2D2 and C2D2. Two mechanisms seem to be applicable to the other 2 primary

processes which give 1,2-butadiene and H2 + C4H4, resp. 2957-97-3 13160-90-2

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 2957-97-3 CAPLUS 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester,

 $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

13160-90-2 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (9CI) (CA INDEX NAME)



L22 ANSWER 35 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:465275 CAPLUS

DOCUMENT NUMBER:

65:65275 65:12123f-q

KIND DATE

ORIGINAL REFERENCE NO.:

TITLE: Preparation of oximes using a silver chromate and (or)

silver dichromate catalyst INVENTOR(S): Young, Vernon V.

PATENT ASSIGNEE(S): Commercial Solvents Corp.

SOURCE: 8 pp. DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION: DATENT NO

| | PAIENI NO. | KIND | DAIL | APPLICATION NO. | DAIL |
|------|---------------------|-----------|--------------|-------------------------|---------------|
| 2270 | US 3267142 | | 19660816 | US 1964-412334 | 19611218 |
| | RITY APPLN. INFO.: | | | US | 19611218 |
| AB | To a suspension of | 17 g. A | gNO3 and 21. | 5 g. ZnO in 400 ml. H20 | were added |
| | solns. of 13 g. (N | 14) 2Cr20 | 7 or 16.2 g. | CaCr2O7 or 15 g. Na2Cr | 207.2H20 or |
| | 15 g. K2Cr2O7 or 10 | g. Cr0 | 3 in 200 ml. | H2O. The solids were | filtered off |
| | and dried at 100°. | Simila | rly prepared | were Ag2CrO4 and Ag2Cr | 207 on |
| | CaCO3, Al2O3, SiO2, | CaO, C | aHPO4, Ca3(P | 04)2, and TiO2. These | catalvsts |
| | were used for the l | nydrogen | ation of nit | roparaffins in MeOH at | 500-1000 psi. |
| | and 135°. Several | examples | are given f | or the reduction of | |
| | nitrocyclohexane wh | nich led | to C6H11NH2 | , C6H11NHOH, and C6H10: | NOH. The |
| | best yields of oxin | ne were | obtained wit | h Ag2Cr04-CaC03 1:1 (23 | .8%) and with |
| | Ag2Cr2O7-ZnO 1:1 (2 | 29.3%). | | - | |
| | | | | | |

APPLICATION NO

DATE

- 14495-41-1
- (Derived from data in the 7th Collective Formula Index (1962-1966))
- RN 14495-41-1 CAPLUS
- CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



L22 ANSWER 36 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1966:465274 CAPLUS

DOCUMENT NUMBER: 65:65274

ORIGINAL REFERENCE NO.: 65:12123f

TITLE:

Isomerization of tetramethyl cis, trans, cis-1,2,3,4-cyclobutanetetracarboxylate

INVENTOR(S): Griffin, Gary W.

PATENT ASSIGNEE(S): American Cyanamid Co.

2 pp.; Division of U.S. 3,139,395 (CA 61, 6937b) SOURCE:

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|----------|--------------|--------------------|----------|
| | | | | |
| US 3253016 | | 19660524 | US 1964-351519 | 19640312 |
| PRIORITY APPLN. INFO.: | | | US | 19640312 |
| AB The disclosure is | the same | but the clas | ims are different. | |

AF

ΙT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

14495-41-1 CAPLUS RN

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA CN INDEX NAME)

1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis, trans, cis- 3999-67-5P,

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, trans, trans, trans-

RL: PREP (Preparation) (preparation of)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

3999-67-5 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 37 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:438196 CAPLUS DOCUMENT NUMBER: 65:38196

ORIGINAL REFERENCE NO.: 65:7072h,7073a

TITLE: Electrolytic oxidation of cyclobutane-1,3-dicarboxylic acids. An electrochemical synthesis of

2,4-dicarbomethoxybicyclobutane

AUTHOR(S): Vellturo, Anthony F.; Griffin, Gary W.

CORPORATE SOURCE: Tulane Univ., New Orleans, LA
SOURCE: Journal of Organic Chemistry (1966), 31(7), 2241-4

SOURCE: Journal of Organic Chemistry (19 CODEN: JOCEAH: ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

LANGUAGE: English
AB Anodic oxidation of trans, trans, trans-1, 3-dicarboxy-2, 4-

dicarbomethoxycyclobutane in the Kolbe manner gives

2,4-dicarbomethoxybicyclobutane. In contrast, electrolysis of

 $\alpha\text{-trux}\textsc{illic}$ acid under similar conditions results in ring contraction and formation of the lactone of

cis, cis-1-carboxy-2-(\alpha-hydroxybenzyl)-3-phenylcyclopropane as the

major product. A cationic mechanism is invoked to explain the difference in behavior exhibited by these cyclobutane-1,3-dicarboxylic acids.

IT 2957-97-3

(Derived from data in the 7th Collective Formula Index (1962-1966)) RN 2957-97-3 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, (1α,2β,3α,4β)- (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L22 ANSWER 38 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:438195 CAPLUS

DOCUMENT NUMBER: 65:38195 ORIGINAL REFERENCE NO.: 65:7072h

TITLE: 1,5,9-Tridehydro-12-annulene

AUTHOR(S): Sondheimer, F.; Wolovsky, R.; Garratt, P. J.; Calder,

I. C.

CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, UK SOURCE:

Journal of the American Chemical Society (1966), 88(11), 2610

CODEN: JACSAT: ISSN: 0002-7863

Journal DOCUMENT TYPE:

LANGUAGE: English

Correction. Isomer B reported (CA 64, 6515e) was shown to be identical

with the title compound 2957-97-3

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 2957-97-3 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester,

 $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

L22 ANSWER 39 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1966:85300 CAPLUS DOCUMENT NUMBER: 64:85300

ORIGINAL REFERENCE NO.: 64:16081g-h,16082a TITLE: Esters of 1,2,3,4-cyclobutanetetracarboxylic acid as

plasticizers for resins and rubbers

INVENTOR(S): Rhum, David; Maggart, Ronald C.; Roper, Robert

PATENT ASSIGNEE(S): Esso Research and Engineering Co. SOURCE:

3 pp. DOCUMENT TYPE: Patent

LANGUAGE: Unavailable FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-----------------------------------|------|----------|----------------------|----------------------|
| US 3236801
ORITY APPLN. INFO.: | | 19660222 | US 1963-255073
US | 19630130
19630130 |

PRIC AR Esters of 1,2,3,4-cyclobutanetetracarboxylic acids are prepared by direct esterification of the appropriate 1,2,3,4-cyclobutanetetracarboxylic acid, dianhydride or acid chloride, by transesterification, or by direct dimerization of a dialkyl maleate or fumarate. When used in amts. of 5-150 parts per 100 parts resin, they give improved low-temperature properties, less volatile loss, and a better compatability-volatility relation. Thus, a mixture of 45 g. tetra-Me 1,2,3,4-cyclobutanetetracarboxylate, 127.5 g. Oxo hexyl alc. and 0.5 g. NaOMe was heated under N to .apprx.140°. After removing most of the alc., the solution was cooled, washed and vacuum stripped to yield tetrahexyl 1,2,3,4-cyclobutanecarboxylate. Fifty parts of this plasticizer was milled into 100 parts of Geon 101 poly(vinyl chloride) containing 2 parts stabilizer. Molded samples gave the following properties (compared with controls containing equal amts. of adipic polyester and dioctyl phthalate): volatility (% plasticizer loss after 7 hrs. at

136°), monomeric tetrahexyl ester 24, adipic polyester 17, dioctyl phthalate 91; % retention of elongation (after 7 hrs. at 136°), monomeric tetrahexyl ester 73, adipic polyester, 76, dioctyl phthalate zero.

7566-44-1, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetrahexyl ester

(vinyl chloride polymers plasticized by)

7566-44-1 CAPLUS RN

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetrahexyl ester (CA INDEX NAME)

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD OS.CITING REF COUNT: 1 (1 CITINGS)

L22 ANSWER 40 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1965:438739 CAPLUS 63:38739

DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 63:6882b-e

TITLE: Electrochemical synthesis of a bicyclobutane

AUTHOR(S): Vellturo, Anthony F.; Griffin, Gary W. CORPORATE SOURCE: Tulane Univ., New Orleans, LA

SOURCE: Journal of the American Chemical Society (1965),

87(13), 3021-2

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Electrolysis of trans, trans, trans-1, 3-dicarboxy-2, 4dicarbomethoxycyclobutane (I), m. 183-4°, under Kolbe conditions

gave 2,4-dicarbomethoxybicyclobutane (II), assumed to be cis, m. 83-5° whose structure was assigned on the basis of its ir and N.M.R. spectra. Further evidence for this structure was obtained by hydrogenation of H over PtO2 to cis-1,3-dicarbomethoxycyclobutane (III), MeO2C(CH2)4CO2Me, and MeO2CCH2CH2CH2CHMeCO2Me. trans,trans,trans=I was prepared by ozonolysis of the di-Me ester of ϵ -truxillic acid and its structure confirmed by conversion to the known trans, trans, trans-1, 2, 3, 4-tetracarbomethoxycyclobutane (IV) on treatment with CH2N2. It was established that I was not identical (ir spectrum and mixed m.p.) with trans, trans, trans-1, 2-dicarboxy-3, 4dicarbomethoxycyclobutane (V), m. 167-70°, prepared by treating dianhydride VI CA 61, 4233e with 2 equivs. of NaOMe. All attempts to prepare trans, trans, trans-I from VI failed.

2957-97-3

(Derived from data in the 7th Collective Formula Index (1962-1966)) 2957-97-3 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (CA INDEX NAME)

```
HO<sub>2</sub>C
                                 OMe
                         CO2H
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OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 41 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1965:438738 CAPLUS

DOCUMENT NUMBER:

63:38738

ORIGINAL REFERENCE NO.: 63:6881g-h,6882a-b

TITLE: Derivatives of tetrahydrodicyclopentadiene in the field of fats. I. Tricyclodecamethanal as starting

material Kaufmann, H. P.; Grothues, B. AUTHOR(S):

CORPORATE SOURCE: Deut. Inst. Fettforsch., Muenster, Germany

SOURCE: Fette, Seifen, Anstrichmittel (1965), 67(4), 249-55

CODEN: FSASAX: ISSN: 0015-038X

DOCUMENT TYPE: Journal LANGUAGE: German

For diagram(s), see printed CA Issue.

Several derivs. of tricyclodecamethanal (I) were prepared and studied. I 2,4-dinitrophenylhydrazone, m. 144°, was obtained in 43% yield by

the usual method. 0.15 mole I in ether solution was treated with dry HCl gas. The mixture was neutralized with K2CO3 and extracted with ether, giving a 50% yield of I diethyl acetal, b11 141-3°. By treating I with 1 and 2 moles, respectively, of malonic acid in a pyridine-piperidine solution,

β-tricyclodecylacrylic acid (II), m. 157°, and

β-tricyclodecylglutaric acid, m. 179°, were obtained. By removing the crystalline II from the reaction mixture, a sirupy isomer of II,

b11 197-200°, could be isolated. From the crystalline II was prepared by the

usual method II anilide (66% yield), m. 163°, whereas the sirupy II vielded 95% II anilide, b5 150-60°, and 84% II Me ester, b10

162-5°. The appearance of the II isomers was studied by their catalytic hydrogenation which yielded a mixture of tricyclodecylpropionic

acids: a sirupy isomer, b6 166-8°, and a crystalline form, m. 81°. This was taken as evidence that the source of the isomerism

lies in the tetrahydrodicyclopentadienyl ring system. Oxidation with KMnO4 of the crystalline II vielded tricyclodecylcarboxylic acid (III), m.

114°, whose anilide, m. 143°, was obtained in 41% yield. The reduction with LiAlH4 of I yielded a viscous mixture of alcs. which could not be resolved, although a well defined 3,5-dinitrobenzoate derivative, m. 71°, was obtained. By treating III with HN3, tricyclodecylamine

(IV), b11 103°, was isolated in 49% yield; IV N-benzoyl derivative, m. 123°, was prepared in 35% yield.

2957-97-3

(Derived from data in the 7th Collective Formula Index (1962-1966)) 2957-97-3 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,3-dimethyl ester, $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (CA INDEX NAME)



L22 ANSWER 42 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1965:82131 CAPLUS

DOCUMENT NUMBER: 62:82131

ORIGINAL REFERENCE NO.: 62:14523b-d TITLE: New routes i

TITLE: New routes into the cis,trans,cis-tricyclo[5.3.0.002.6]decane series

AUTHOR(S): Buchta, Emil; Merk, Wolfgang

CORPORATE SOURCE: Univ. Erlangen, Nuremberg, Germany

SOURCE: Naturwissenschaften (1965), 52(6), 130

CODEN: NATWAY; ISSN: 0028-1042

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB I (R = CO2Et), m. 144-5°, reduced with LiAlH4 in dry

tetrahydrofuran gave I (R = CH2OH, m. 62-4°, which with p-MeC6H4SO2Cl yielded I (R = p-MeC6H4SO2CH2) (II), m. 126.5-7°. II

with NaCH(CO2Et)2 in refluxing xylene gave 82% III (R1 = R2 = R3 = R4 = CO2Et) (IV), b0.03 $185-7^{\circ}$ m. $66-7.5^{\circ}$ (petr. ether). IV

reduced with LiAlH4 in dry tetrahydrofuran gave 75% III (R1 = R2 = R3 = R4

= CH2OH), m. 242-4°. Saponification of IV have crude III (R1 = R2 = R3 = R4 = CO2H), which decarboxylated at 210-20° yielded a mixture of III (R1 = R3 = H, R2 = R4 = CO2H) and III (R1 = R4 = H, R2 = R3 = CO2H), m.

250-70° (sealed capillary).

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 14495-41-1 CAPLUS

RN 14495-41-1 CAPLUS

N 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

IT 1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis,trans,cis-RL: PREP (Preparation)

(preparation of) RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)



L22 ANSWER 43 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1965:82130 CAPLUS

DOCUMENT NUMBER: 62:82130

ORIGINAL REFERENCE NO.: 62:14523a-b

TITLE: Isomerization via transannular enolate anion

AUTHOR(S): Fukunaga, Tadamichi

CORPORATE SOURCE: E. I. du Pont de Nemours & Co., Wilmington, DE SOURCE: Journal of the American Chemical Society (1965),

87(4), 916-17 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English For diagram(s), see printed CA Issue.

A base-catalyzed isomerization reaction of the half-cage ketone (I) to the iso-half-cage ketone (II) was reported. I with tert-BuOK in tert-BuOH in a sealed tube at 250° quant. gave II, containing .apprx.4% I. The ir

and N.M.R. spectra of II were discussed. 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



L22 ANSWER 44 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1965:73878 CAPLUS

DOCUMENT NUMBER: 62:73878

ORIGINAL REFERENCE NO.: 62:13056c-h,13057a-b

Synthesis of cyclobutane derivatives from unsaturated fatty acid esters. Photochemical reactions of muconic

acid dimethyl ester and sorbic acid methyl ester

AUTHOR(S): Kaufmann, Hans P.; Sen Gupta, Achintya K. CORPORATE SOURCE:

Deut. Inst. Fettforsch., Muenster, Germany SOURCE:

Justus Liebigs Annalen der Chemie (1965), 681, 39-44

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal LANGUAGE: German

For diagram(s), see printed CA Issue.

AB Irradiation of muconic acid di-Me ester (I) and sorbic acid Me ester (II) in

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C6H6 in the presence of Ph2CO gave cyclobutane derivs. along with
     cis,-trans isomers. trans,trans-I (10.5 g.) suspended in 1 1. absolute C6H6
     containing 2 g. Ph2CO irradiated 40 h. at 20° with a Hg high pressure
     burner (200-w.) with stirring and exclusion of O in a Jena glass flask,
     and the solution worked up gave 2.2 g. unchanged trans, trans-I, m.
     157°, 1.99 g. Ph2CO, m. 48°, 142 mg. cis, cis-I, m.
     75°, 201 mg. solid, m. 55°, 210 mg. cis,trans-I, m.
     75°, 658 mg. trans, trans-I, m. 158°; 28 mg. unidentified
     oil, 6.92 g. III and IV, oil, and 130 mg. unidentified oil. Cis,cis-I was
     (III) (R = CO2Me, R1 = CH:CHCO2Me) (V) (R = CO2H, R1 = CH:CHCO2H) (VI) (R = R1
     = CO2H) (VIII) (R = CO2Me, R1 = CH: CHMe (X) (R = Me, R1 = CH: CHCO2Me) (IV) (R
     = R2 = CO2Me, R1 = R3 = CH:CHCO2Me) (VII)(R = R2 = CO2H, R1 = R3 =
     CH:CHCO2H) (IX)(R = Me, R1 = CH:CHMe, R2 = CO2Me, R3 = CH:CHCO2Me) saponified
     to cis, cis-muconic acid, m. 184°, which treated with H2SO4 gave
     \gamma-carboxymethyl-\delta\alpha, \beta-crotonolactone, m.
     110°. cis,cis-I heated 4 h. in H2O gave cis,trans-I, m. 75°.
     cis,-trans-I was converted into trans, trans-I, m. 158°, by
     irradiating its MeOH solution in the presence of a trace of iodine. The
     III-IV mixture above in 50 cc. Et20 kept 16 h. at -30° and the precipitate
     (3.39 q.) filtered [the filtrate (A) was kept] and recrystd. twice from
     MeOH gave III, m. 43°. III (1 g.) refluxed 8 h. with 20 cc. 10%
    MeOH-NaOH, the solution diluted with H2O and extracted exhaustively with
EtOAc, the
    extract dried and evaporated in vacuo, and the residue (0.6 g. V) in 150 cc. 2%
     aqueous NaOH treated portion-wise with KMnO4 during .apprx.4 h. at the b.p.
     and worked up gave 185 mg. trans, trans, trans-VI, m. 260-4° (Me2CO
     petr. ether); tetra-Me ester (via CH2N2) m. 126-7° (C6H6-petr.
     ether). Filtrate A gave trans, trans, trans-IV, m. 57-8° (aqueous
     MeOH), saponified (8 h. reflux with 10% MeOH-NaOH) to trans, trans, trans-VII,
     m. 245° (decomposition) (EtOAc-Me2CO-petr. ether), which (0.5 g.)
     oxidized with KMnO4 as above gave 185 mg. trans, trans, trans-VI, m.
     260-4° (Me2CO-petr. ether). trans, trans-II (20 g.) in 2 1. absolute
    C6H6 containing 5 g. Ph2CO irradiated like I 100 h. at 20° with
     stirring and worked up gave 14.7 g. unchanged crude trans, trans-II, 5.0
     g. Ph2CO, trans, trans, trans-VIII (1.88 g. crude), colorless oil, n20D
     1.4796, mol. weight (cryoscopic in C6H6) 246, saponification number 438, 441
    [trans, trans, trans-VIII (1 g.) saponified by alkali and the oily saponification
    product oxidized with alkaline KMnO4 as above gave 168 mg.
    trans, trans, trans-VI, m. 262°], trans, trans, trans-IX (0.99 g.
    crude), colorless oil, n20D 1.4841, mol. weight (cryoscopic in C6H6) 249,
    saponification number 440.9 [trans, trans, trans-IX (0.5 g.) saponified and
subsequently
     oxidized with KMnO4 gave 43 mg. trans, trans, trans-VI], and
     trans, trans, trans-X (2.51 g. crude), b0.15 89-92°, mol. weight
     (cryoscopic in C6H6) 248.6, saponification number 442.4, which (1 q.)
saponified and
     oxidized with KMnO4 gave 40 mg, trans, trans, trans-VI, m. 260-4°.
     14495-41-1
        (Derived from data in the 7th Collective Formula Index (1962-1966))
     14495-41-1 CAPLUS
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1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA

INDEX NAME)

RN

CN

3999-67-5P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, trans, trans, trans-RL: PREP (Preparation) (preparation of)

3999-67-5 CAPLUS

CN 1.2.3.4-Cvclobutanetetracarboxvlic acid, tetramethyl ester. $(1\alpha, 2\beta, 3\alpha, 4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 45 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1965:73877 CAPLUS

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.:

62:73877 62:13056b-c

TITLE:

Substituted cyclopropenones

AUTHOR(S):

Breslow, Ronald; Altman, L. J.; Krebs, Adolf; Mohacsi, Erno; Murata, Ichiro; Peterson, Ruth A.; Posner, Judd

CORPORATE SOURCE:

Columbia Univ. Journal of the American Chemical Society (1965),

SOURCE:

87(6), 1326-31

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 62:73877

- AR Dipropylcyclopropenone (I) may be synthesized by addition of dichlorocarbene to dipropylacetylene; under some conditions a cyclobutenone derivative is also formed. Elimination of HBr from bis(bromobuty1) ketone also affords I, along with a cyclopentenone derivative The same HBr elimination route has been used to prepare dibutylcyclopropenone, cycloheptenocyclopropenone, and cycloundecenocyclopropenone. Properties and reactions of these compds. and synthetic approaches to other cyclopropenones are described.
- 14495-41-1 (Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS CN

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

THERE ARE 18 CAPLUS RECORDS THAT CITE THIS OS.CITING REF COUNT: 1.8 RECORD (18 CITINGS)

L22 ANSWER 46 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1965:15312 CAPLUS DOCUMENT NUMBER: 62:15312

ORIGINAL REFERENCE NO.: 62:2769b-e

TITLE: Photochemical studies, II. Structure of the

photodimers of carbostyril and N-methylcarbostyril

AUTHOR(S): Buchardt, O.

Univ. Copenhagen

SOURCE: Acta Chemica Scandinavica (1964), 18(6), 1389-96

CODEN: ACHSE7; ISSN: 0904-213X

DOCUMENT TYPE: Journal English

LANGUAGE:

For diagram(s), see printed CA Issue.

cf. CA 59, 13946a. Chemical and spectroscopic evidence show that the dimers of carbostyril and N-methylcarbostyril have the

trans-head-head-cyclobutane structures (I, R = H and I, R = Me), resp. The dimers I (R = H) and I (R = Me) were ozonized and oxidized with H2O2

and the products were hydrolyzed with dilute HCl and methylated directly to yield, in both cases, tetramethyl cis-trans-cis-

cyclobutanetetracarboxylate. Attempts to methylate I (R = H) to give I (R = Me) were unsuccessful so that the two compds. were interrelated as

follows. I (R = Me) was reduced with LiAlH4 in Et2O to give II (R = Me), m. 184-5°; monomethiodide m. 185-6°; dimethiodide m.

260-70°. Reduction of I (R = H) with LiAlH4 gave II (R = H), m. 125-6°, which on treatment with MeI and then aqueous KOH gave II (R = Me). The trans-head-head configuration in both compds. was established by

measurement of dipole moments in C6H6 [2.53 D. for II (R = H) and 5.28 D. for I (R = Me)].

14495-41-1 (Derived from data in the 7th Collective Formula Index (1962-1966))

RM 14495-41-1 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

1032-95-7P, 1,2,3,4-Cvclobutanetetracarboxvlic acid, tetramethvl ester, cis, trans, cis-RL: PREP (Preparation)

(preparation of)

1032-95-7 CAPLUS RN

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L22 ANSWER 47 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1964:440150 CAPLUS

DOCUMENT NUMBER: 61:40150

ORIGINAL REFERENCE NO.: 61:6937c-d

TITLE: Purification of nitrocyclohexane

INVENTOR(S): Chandler, Ollie W.
PATENT ASSIGNEE(S): Commercial Solvents Corp.

PATENT ASSIGNEE(S): Commercial Solvents
SOURCE: 2 pp.

DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|------|
| | | | | |
| US 3132183 | | 19640505 | US | |

AB To a 600 g, portion of the crude product from the nitration of cyclohexane consisting of 94.7% nitrocyclohexane (I) with cyclohexanene, cyclohexal nitrate, and nitrocyclohexane as impurities, was added 100 g. of 96% H2SO4 at such a rate as to give a final temperature of 70°. The mixture was held at 70° with thorough agitation 3 hrs. After the addition of 100 ml.

of H2O, the mixture was steam distilled at atmospheric pressure to give $540\ \mathrm{g}$ oduct

containing 99.5% I. Cf. Smiley, CA 53, 2243b.

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

L22 ANSWER 48 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1964:440149 CAPLUS DOCUMENT NUMBER: 61:40149

ORIGINAL REFERENCE NO.: 61:40149

TITLE: Photodimerization of fumaric acid derivatives

INVENTOR(S): Griffin, Gary W.

PATENT ASSIGNEE (S): American Cyanamid Co. SOURCE: 2 pp.

DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------|------------------|------|----------|-----------------|----------|
| | | | | | |
| | US 3139395 | | 19640630 | US 1961-81224 | 19610109 |
| PRIOR | RITY APPIN. INFO | | | IIS | 19610109 |

AB Cyclobutanetetracarboxylic acid or their Me esters are made by subjecting a solid layer of di-Me fumarate to light waves of 1750-4000 A. The cyclobutane dianhydride can be made by a similar method from maleic anhydride irradiated in the solid state. Thus, a solution of di-Me fumarate in CH2Cl2 is deposited on the inside wall of a glass cylinder, the CH2Cl2 evaporated, and a lamp inserted in the cylinder. Irradiation is maintained for 24 hrs. with cooling to give 59% the tetramethyl ester of cis, trans, cis-1,2,3,4-cyclobutanetetracarboxylic acid, m. 144-5°. Also prepared were cis, trans, cis-1, 2, 3, 4-tetracyanocyclobutane, m. 250° (decomposition), 1,2,3,4-cyclobutanetetracarboxylic acid dianhydride, and tetra-Me trans, trans, trans-1, 2, 3, 4-cvclobutanetetracarboxylate, m. 123-5°.

14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

14495-41-1 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

1032-95-7P, 1,2,3,4-Cvclobutanetetracarboxvlic acid, tetramethvl ester, cis, trans, cis- 3999-67-5P,

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, trans, trans, trans-

RL: PREP (Preparation)

(preparation of) 1032-95-7 CAPLUS

RN CN 1,2,3,4-Cvclobutanetetracarboxvlic acid, tetramethvl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

RN 3999-67-5 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, (1α,2β,3α,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L22 ANSWER 49 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1964:425032 CAPLUS

DOCUMENT NUMBER: 61:25032

ORIGINAL REFERENCE NO.: 61:4233e-h,4234a-b

TITLE: Reductive cleavage of tetrasubstituted cyclobutanes:

possible examples of homolytic fragmentations
AUTHOR(S): Griffin, G. W.; Hager, R. B.

CORPORATE SOURCE: Yale Univ.

SOURCE: Rev. Chim., Acad. Rep. Populaire Roumaine (1962),

7(2), 901-6 DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 57, 16417d. Several possible examples of homolytic fragmentation of tetrasubstituted cyclobutanes were considered, employing Mg-MgI2 in THF (in ether-benzene the mixture was inactive) and Na in liquid NH3 for the

reductive cleavage. Reduction of trans,trans,trans-1,2,3,4tetrabenzoylcyclobutane (Ia) with Mg-MgI2 and subsequent hydrolysis gave

high yields (61%) of dibenzoylethane instead of the expected intramol. pinacol reduction, with a dienolate (II) presumed as initial product.

Reduction

of trans, trans, trans-1, 2, 3, 4-tetracarbomethoxycyclobutane (Ib) with Na and hydrolysis gave only di-Me succinate (25% yield) while similar treatment of the cis, trans, cis-1, 2, 3, 4-tetracarbomethoxycyclobutane (III) gave the same di-Me succinate (23%). Similar treatment of the tetraketone (Ic) gave 2,5-hexanedione (53%) as major product and of the dioxodiester (Id), both 2,5-hexanedione (24%) and di-Me succinate (4%) and some Me levulinate (IV) (12%). Details were presented on the preparation of (Ic) and the unusual cage dianhydride (VI). The tetraketone (Ic), m. 139-40°, was prepared in 57% yield from the tetradiazoketone (V) by the action of HI in CHCl3. VI, m. 280° (decomposition), was prepared in 65% yield by treatment of Ie with Ac20. Methanolysis of VI afforded Iq, and conversion of the latter through its acid chloride and diazoketone gave the trans, trans, trans-1, 2-diacety1-3, 4-dicarbomethoxycyclobutane (Id), m. 81-2°, in 83% yield from VI. Dibenzoylethane was cleaved under similar conditions to give a low yield of acetophenone and 1,2-diphenyl-1,2-dihydroxycyclobutane, m. 147-50°. A photochem. reductive cleavage of Ia to dibenzoylethane was accomplished by irradiating in benzene in Pyrex glass vessels in the presence of benzophenone as photosensitizer. The same photosensitizer was used for photochem. reduction of dibenzoylethylene, using iso-PrOH, cyclohexane, or SnBu3H as H donors. Several possible interpretations were presented on the mechanism of the apparently general cleavage reaction. 28 refs.

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

IT 1032-95-7, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis,trans,cis- 3999-67-5,

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, trans,trans,trans-

(reductive cleavage of)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

RN 3999-67-5 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\beta,3\alpha,4\beta)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 1 T

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 50 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1964:425031 CAPLUS DOCUMENT NUMBER: 61:25031

ORIGINAL REFERENCE NO.: 61:4233d-e

TITLE: Cyclobutane compounds. I. Formation of a four-membered

ring during the electrophilic addition of hydrogen bromide to allene

AUTHOR(S): Griesbaum, Karl

CORPORATE SOURCE: Esso Res. & Eng. Co., Linden, NJ

SOURCE: Journal of the American Chemical Society (1964),

86(11), 2301-3

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB The reaction of equimolar amts. of HBr and CH2:C:CH2 (I) produced (yields

from gas-liquid chromatography) 13% CH2:CBrMe, 35% Me2CBr2, 44% trans-1,3-dibromo-1,3-dimethylcyclobutane (II), m. 54-5°, δ

2.13 (singlet) and 3.19 (singlet) p.p.m., and 8%

cis-1,3-dibromo-1,3-dimethylcyclobutane (?). Reduction of II with Bu3SnH

produced a mixture of cis- and trans-1,3-dimethylcyclobutane. The formation of II represented the first example of a cationically induced

cyclodimerization of I.

T 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966)) RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 51 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1964:52579 CAPLUS DOCUMENT NUMBER: 60:52579

ORIGINAL REFERENCE NO.: 60:9210e-h,9211a

TITLE: Investigations in the cyclobutane series. XII. Two

stereoisomeric dimers of cyclobutadiene

AUTHOR(S): Avram, Margarete; Dinulescu, Ilie G.; Marica, Elise;
Mateescu, Georg; Sliam, Elvira; Nenitzescu, Costin D.
CORPORATE SOURCE: Acad. R. V. R., Bucharest, Rom.

CORPORATE SOURCE: Acad. R. V. R., Bucharest, Rom. SOURCE: Chemische Berichte (1964), 97(2), 382-9

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 60:52579
GI For diagram(s), see printed CA Issue.

AB The elimination of Cl from cis-3,4-dichlorobutene (I) with Na-Hg in Et2O yielded syn-tricyclo(4.2.0.02.5)ccta-3,7-diene (II). I with Li-Hg gave similarly predominantly the anti isomer (III) of II. The ozone cleavage and several derivs. of II and III are described. I in Et2O shaken 40 hrs.

with 0.5% Na-Hg, and the solution treated with saturated aqueous AgNO3 yielded 46-51%

AgNO3 complex (IV) of II, m. 138-40°. IV shaken at 0° with

saturated aqueous NaCl yielded 65-9% II, b40 45°, containing 2-3% cyclooctatetraene (V). I in Et2O shaken 8-10 hrs. with 0.5% Li-Hq, and the solution shaken with saturated aqueous AqNO3 gave 55% AqNO3-complex (VI) of III, m. 152° (EtOH). VI shaken at 0° with saturated aqueous NaCl yielded 51% III, b40 40°, m. .apprx.-15°. II in 90% AcOH ozonized 8 hrs. and treated 36 hrs. with 30% H202 yielded 77% all-cis-1,2,3,4-tetracarbomethoxycyclobutane (VII), m. 202°. III yielded similarly 85% cis-trans-trans-isomer of VII, m. 147° (C6H6). III in MeOH hydrogenated over 30% Pd-C vielded anti-tricyclo[4.2.0.02.5]-octane (VIII), b30 53°. VIII heated 8-10 hrs. under argon at 150° gave 39% dimeric 1,5-cyclooctadiene (IX), m. 121° (sealed capillary), and a liquid hydrocarbon C8H12, isolated as the yellow PdCl2 complex, m. 205-10° (decomposition) (AcOH). II hydrogenated similarly gave the syn isomer (X) of IX, which, rearranged thermally, yielded 12.5% IX. II in CH2C12 treated at 0° with Br gave 77% 3,4,7,8-tetra-Br derivative (XI) of X, pale yellow viscous liquid, which deposited on standing a hexabromide, m. 168° (MeOH). III yielded similarly 94% 3,4,7,8-tetra-Br derivative (XII) of XI, m. 172° (heptane). XII in Et20 shaken 10 hrs. with 0.5% Li-Hq gave 52% III. XII in PhCl heated 2 hrs. at 130-40° gave 77.5% C8H8Br4, m. 136-7° (AcOH). XII and 2.5-diphenvl-3.4-benzofuran (XIII) in Et20 shaken 16 hrs. with 0.5% Li-Hg, the precipitate treated with maleic anhydride, and the product refluxed 15 min. with 5% KOH-MeOH vielded 43% adduct, m. 252°. 1,2,3,4-Tetrabromocyclobutane, XIII, and 0.5% Li-Hg in Et20 yielded similarly 6% adduct, m. 288-90° (AcOH). The infrared absorption spectra of II, III, VIII, and X are recorded. 31351-41-4P RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Investigations in the cyclobutane series, XII, Two stereoisomeric dimers of cyclobutadiene)

Relative stereochemistry.

31351-41-4 CAPLUS

 $(1\alpha, 2\alpha, 3\alpha, 4\alpha)$ - (9CI) (CA INDEX NAME)

RN

IIT 14495-41-1P, 1,2,3,4-Cyclobutanetetracarboxylic acid,
 tetramethyl ester, stereoisomers
 RL: PREP (Preparation)
 (preparation of)
RN 14495-41-1 CAPUUS

N 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester,

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L22 ANSWER 52 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN 1963:435251 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

59:35251

ORIGINAL REFERENCE NO.: 59:6273e-h,6274a

TITLE: The tricyclo[5.3.0.02,6]decane system. Photodimers of cyclopentenone

AUTHOR(S): Eaton, Philip E.

CORPORATE SOURCE: Univ. of California, Berkelev

SOURCE: Journal of the American Chemical Society (1962),

84(12), 2344-8 CODEN: JACSAT: ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable OTHER SOURCE(S): CASREACT 59:35251

For diagram(s), see printed CA Issue.

The photodimers of cyclopentenone (I) were shown to be II and III. II was converted by 2 paths into cis, trans, cis-tricyclo[5.3.0.02,6]deca-4,9-diene-3,8-dione (IV). The cis,trans,cis assignment for II, III, and other derivs. was based partially on NMR data. Irradiation of I 24 h. with a Hg arc lamp through Pyrex glass gave 43-49% II, m. 125-6.5° (sublimed at 0.5 mm. and crystallized from CH2C12-hexane) and 37-45% III, m. 66-7° (hexane). Wolff-Kishner reduction of II and III gave cis, trans, cis-tricyclo[5.3.0.02,6]decane, identified by gas chromatog. II with monoperoxyphthalic acid in ether yielded 60% V, m. 156-7° (C6H6-CCl4). III similarly gave 55% VI, m. 103-5°. Methanolysis of V over polystyrenesulfonic acid resin was accomplished without rearrangement to give. putative 1,3-bis(2-carbomethoxyethy1)cyclobutane-2,4-diol, λ 2.87 (OH), 5.77 μ (ester CO), which reverted to V on attempted distillation VI similarly vielded 1,2-bis(2-carbomethoxyethyl)cyclobutane-3,4-diol, oxidizable with Pb(OAc)4. II with isopropenyl acetate and p-MeC6H4SO3H gave 58 (crystallized from hexane) or 26% (chromatographed on neutral Al203) dienol acetate (VII), m. 95-6°, which with Na2CO3 in aqueous MeOH reverted to II. VII (16.00 g.) in CH2C12 at -65° with 20.65 g. Br vielded 13.4 g. putative tetrabromide, which with tert-BuOK in tert-BuOH refluxed overnight yielded 36% IV, m. 231-3°. II with (HOCH2)2 and HCl gave 91% bis(ethylene ketal), m. 143-3.5°, which (54.5 g.) in THF with 174 g. pyridinium bromide perbromide yielded 54% dibromo derivative (VIII), m. 200° (decomposition). VIII with tert-BuOK in Me2SO (not in tert-BuOH) gave 84% bis(ethylene ketal), m. 177-8° (hexane), of IV, which with 0.1N HCl in THF yielded 91% IV. Hydrogenation of IV in AcOH over Pd-C

14495-41-1 (Derived from data in the 7th Collective Formula Index (1962-1966))

143-4°. NMR spectra of IV-VI were given.

RN CN

14495-41-1 CAPLUS 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

yielded II. IV in aqueous AcOH with ozone and then H2O2 followed by treatment with CH2N2 afforded 28% cis, trans, cis-tetracarbomethoxycyclobutane, m.

IT 1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl
 ester, cis,trans,cisRL: PREP (Preparation)
 (preparation of)

RN 1032-95-7 CAPLUS
CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, (10,20,30,40)- (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L22 ANSWER 53 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:435250 CAPLUS DOCUMENT NUMBER: 59:35250

ORIGINAL REFERENCE NO.: 59:6273a-e

TITLE: Behavior of norbornadiene and its 7-alkoxy derivatives towards organolithium reagents

AUTHOR(S): towards organolithium reagents
Wittig, Georg; Otten, Joachim
CORPORATE SOURCE: Univ. Heidelberg, Germany

SOURCE: Tetrahedron Letters (1963) 601-6 CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB cf. CA 55, 8455c. Treatment of norbornadiene (I) in Et20 with PhLi under various conditions gave the metalated product (II), the 2 addition compds. (III, IV, R = Li, R' = Ph) and dimeric norbornadiene, bl6 121-4°, m. 33°, consisting of a mixture of 2 isomeric compds. The reaction of I with organolithium compds., R'Li, took place relatively slowly, in days at room temperature and in 24 hrs. at 70° and was still more retarded in petr. ether. I treated 6 days with Me2CHLi in petr. ether at 20° and the mixture hydrolyzed yielded 50% IV (R = H, R' = Me2CH) together with 34% I. Similarly, I treated 2 days in petr. ether at 20° with Me3CHLi gave 62% IV (R = H, R' = Me3C) and unchanged I. On the contrary, the addition of R'Li in petr. ether at -20° and hydrolysis of the precipitated material yielded 87% product (VII, R = CMe3, R'

=

Me2CH), b13 91°, n20D 1.4558, and 91% VII (R = CMe3, R' = Me3C), b13 106°, n20D 1.4616. The mixture prior to hydrolysis heated 2 hrs. at 100° gave VIII (R = Me2CH) (IX), b60 76°, n25D 1.4661, and 60% VIII (R = Me3C), b20 64°, n20D 1.4718. IX hydrogenated in the presence of prereduced PtO2 with adsorption of 1.98 moles H gave 7-isopropylnorbornane, b. 165°, n20D 1.4580, identical with material prepared by treatment of 7-bromonorbornane with Me2CHBr and Na. Similarly, V (R = Me) treated with Me2CHLi in petr. ether gave an adduct, hydrolyzed to yield 94% VII (R = Me, R' = Me2CH). The mixture heated prior to hydrolysis gave about 50% VIII (R' = Me2CH). V(R = Me3C) (VI) in moist Et20 saturated with dry HCl gave 68% VIII (R' = Cl), b13 46°, n25D 1.5060, m. -16 to -14°, refluxed 4 hrs. in MeOH to give 68% V (R = Me), b18 44°, n20D 1.4792. VI treated with MeOH or EtOH in the presence of a trace of HClO4 yielded 66% V (R = Me) and 82% V (R = Et), resp. The structure of the 7-substituted norbornadienes was conformed by the nuclear magnetic resonance signals for olefin H, bridgehead H, bridge H, and other H atoms: VIII, R = Me2CH, 3.27, 3.49, 6.64, 7.80-8.90, 9.22, 9.31; VIII, R = Me3C, 3.14, 3.60, 6.58, 7.58, 9.21; VIII, R = C1, 3.26, 3.40, 6.38, 5.83; V, R = Me, 3.45, 3.59, 6.54, 6.88; V, R = Et, 3.44, 3.59, 6.38-6.92, 8.93. The above observations suggest that the reactions take place through the 7-norbornadienyl cation (Winstein and Ordronneau, CA 55, 4383i).

IT 14495-41-1

RN

(Derived from data in the 7th Collective Formula Index (1962-1966)) 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L22 ANSWER 54 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:72985 CAPLUS

DOCUMENT NUMBER: 58:72985 ORIGINAL REFERENCE NO.: 58:12431q-h

TITLE: The photodimerization of monomethyl fumarate

AUTHOR(S): Sadeh, T.; Schmidt, G. M. J.

CORPORATE SOURCE: Weismann Inst. Sci., Rehovoth, Israel

SOURCE: Journal of the American Chemical Society (1962), 84, 3970

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Ultraviolet irradiation of a powdered sample of monomethyl fumarate yielded the dimer (I), m. 153-4°. Treatment with SOC12 gave its anhydride, m. 144°. Treatment of both the material and its anhydride with methanolic RCl gave tetramethyl cyclobutane-1,2,3,4-tetracarboxylate m. 144-5°. The conformation of the dimer of monomethyl fumarate was therefore established as having symmetry m, the two acid groups being cis to each other and trans to the two ester groups.

IT 14495-41-1P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (The photodimerization of monomethyl fumarate)

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L22 ANSWER 55 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:473604 CAPLUS DOCUMENT NUMBER: 57:73604

ORIGINAL REFERENCE NO.: 57:14619b-d

TITLE: Mechanism of formation of basic amino acids

(ornithine) and hydroxyamino acids (serine, homoserine) by photochemical synthesis

AUTHOR(S): Ferrari, G.; Passera, C.

CORPORATE SOURCE: Univ. Padua, Italy
SOURCE: Photochemistry and Photobiology (1962), 1, 155-8

CODEN: PHCBAP; ISSN: 0031-8655

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Dicarboxylic diamino acide, monocarboxylic diamino acide, and hydroxyamino acide were synthesized in a study of the action of ultraviolet rays on diluted solns. of inorg. N compds. and ternary organic substances. Hydroxyamino acide are formed by recombination of OH radicals from H202 with amino-group-containing radicals from primary amino acids. a, 8-Diaminoadipic acid, arising by recombination of amino-group-containing radicals from aspartic acid, yields ornithine by

discussed.

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

L22 ANSWER 56 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:473603 CAPLUS

DOCUMENT NUMBER: 57:73603 ORIGINAL REFERENCE NO.: 57:14619a-b

Synthesis of y-keto acids by photochemical TITLE:

reaction

AUTHOR(S): Odaira, Yoshinobu; Tominaga, Tamotsu; Pak, Cheng King;

Tsutsumi, Shigeru

SOURCE: Technology Reports of the Osaka University (1962),

12(Nos. 488-507), 193-7

CODEN: TROUAI; ISSN: 0030-6177

DOCUMENT TYPE: Journal

LANGUAGE:

Unavailable

The photochem. addition reactions of some aldehydes and di-Me fumarate(I) and maleate (II) were studied. Thus, 4-oxoheptanoic acid was prepared from 2 moles butyraldehyde and 1 mole II, exposed to a lowpressure Hg lamp at

room temperature for 100 hrs. Increase in the mole ratio of aldehyde to ester increased the formation of the 1:1 ketodiester adduct except in the case of HCHO. Irradiation of I in the solid state yielded a photodimer

identified as cis, trans, cis-1, 2, 3, 4-tetracarbomethoxycydobutane. ΙT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966)) RN 14495-41-1 CAPLUS

1,2,3,4-Cvclobutanetetracarboxvlic acid, 1,2,3,4-tetramethvl ester (CA CN INDEX NAME)

1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis, trans, cis-

RL: PREP (Preparation)

(formation by irradiation of di-Me fumarate)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 57 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1962:442569 CAPLUS

DOCUMENT NUMBER: 57:42569 ORIGINAL REFERENCE NO.: 57:8446b-i,8447a-d

TITLE: Four-membered ring systems by photosensitized

symmetrical and mixed cycloaddition

AUTHOR(S): Schenck, Guenther Otto; Hartmann, Willy; Mannsfeld,
Sven Peter; Metzner, Wolfgang; Krauch, Carl Heinrich
CORPORATE SOURCE: Max-Planck-Inst. Kohleforschung, Muehlheim, Germany

SOURCE: Bet. (1962), 95, 1642-7

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 57:42569

Dienophiles, such as derivs, of maleic anhydride (I) and judene (II), and cyclic dienes, such as furan, can be condensed to cyclobutane derivs, by photosensitized cycloaddn. according to the principle of the purely biradical substratetransfer. 2,3-Dimethylmaleic anhydride (III) (3.15 g.) and 1.5 g. BzPh in 150 cc. C6H6 irradiated 6 hrs. at 8°, and the precipitate (1.92 g.) sublimed at 230°/0.3 mm. yielded the dianhydride (IV) of tetramethy1-1,2,3,4-cyclobutanetetracarboxylic acid (V), m. from 380° (decomposition and regeneration of III). A similar run but without the BzPh gave during 6 hrs. 0.3 g. IV. IV (0.5 g.) in 50 cc. 30% NaOMe-MeOH refluxed 3 hrs. and treated with 10 cc. Me2SO4 yielded 0.62 q. tetra-Me ester of V, in. $106-8^{\circ}$ (sublimed at $100^{\circ}/0.3$ mm.). 2-Me derivative (20.75 g.) of I and 1.4 g. BzPh in 150 cc. dioxane irradiated 18 hrs. at 10° gave 5.2 g. dianhydride (VI) of dimethylcyclobutanel, 2, 3, 4-tetracarboxylic acid (VII), m. above 350° (decomposition) (sublimed at 280° /0.1 mm.); a similar run without BzPh did not give VI. VI (0.96 g.) in 50 cc. 30% NaOMeMeOH refluxed 6 hrs., acidified with dilute H2SO4, and extracted with Et2O, and the extracted treated with CH2N2-Et2O gave 1.1 g. tetra-Me ester of VII, m. 73-3.5° (sublimed at 60°/ 0.1 mm.). I (29.9 g.) and 2.8 g. BzPh in 150 cc. dioxane irradiated 6 hrs. at 18° gave 1.7 g. cis-trans-cis-cyclobutanel, 2, 3, 4-tetracarboxylic acid dianhydride (VIII), m. 300° (decomposition) (sublimed at 280°/0.1 mm.); a similar run without BzPh yielded 0.9 g. VIII. 2,3-Dimethylmaleimide (IX) (5 g.) and 1.8 g. BzPh in 250 cc. C6H6 irradiated 16 hrs. at 10° yielded 4.2 g. diimide (X) of V, m. 350 °(decomposition) (dioxane), 0.42 g. unchanged IX, and 1.64 g. BzPh; a similar run without BzPh did not give X. N-Phenylmaleimide (XI) (8.7 g.) and 1.8 g. BzPh in 150 cc. dioxane irradiated 24 hrs. at 15° yielded 4.8 g. di(N-phenylimide) (XII) of V, m. 342° (sublimed at 270°/0.1 ram.), 3.6 g. unreacted XI, and 1.66 g. BzPh; a similar run without BzPh did not give XII. N-Cyclohexylmaleimide (XIII) (5.4 g.) and 1.8 g. BzPh in 150 cc. dioxane irradiated 24 hrs. at 15° gave 1.4 g. di(N-cvclohexvlimide) (XIV) of V, m. 293-5° (sublimed at 220° /0.1 mm.), 3.6 g. unchanged III, and 1.66 g. BzPh; a similar run without BzPh did not give X1V. II (20.3 g.) and 3 g. BzPh in 150 cc. C6H6 irradiated 20 hrs. at 15° and evaporated, and the residue chromatographed on silica gel vielded 20 g., cyclobuta [1,2-a:-3,4-a' or 4,3-a']diindene (XV), m. 113° (Me2CO), b0. 134-5°; a similar run without PhBz did not yield XV. III (20 g.) and 2 g. BzPh in 150 cc. furan irradiated 48 hrs. at 10° and concentrated gave 10.6 g. anhydride (XVI) of 6,7-dimethyl-4-oxabicyclo[3.2.01]-2-heptene-6,7-dicarboxylic acid (XVII), m. 153° (sublimed at 100°/0.1 mm.) XVI (1.02 g.) in 15 cc. dioxane hydrogenated under ambient conditions over Raney Ni gave 1.0 g. heptane analog of XVI, m. 120-1 ° (sublimed at 60°/12 mm.). XVI (0.92 g.) in CH2-N2 Et20 containing a small amount EtOH kept 1 hr. and evaporated yielded the di-Me ester (XVIII) of XVII, b0. 95-105° n20D 1.4762, d20 1.157. XVI (0.5 g.) in 40 cc. CHC13, treated at -30° with Br-CHCl3 until the yellow color persisted and evaporated left deliquescent crystals of the unstable 25,35-dibromide (XIX) of XVI. The XIX chromatographed with C6H6 on moist silica gel gave 2ξ-bromo-3ξ-hydroxy-6,7-dimethyl4-oxabicyclo [3.2.0] beptane -6,7-dicarboxylic acid anhydride, m. 183-5°. XVI (2.73 g.) in 50 cc. MeOH containing 5 drops concentrated H2SO4 refluxed 5 hrs., diluted with

H2O, neutralized with aqueous NaOH, and evapd, in vacuo, and the residue chromatographed on silica gel gave 2.5 g. di-Me 3-methoxy-6, 7-dimethy1-4-oxabicyclo [3.2.0] heptane-6,7dicarboxylate, b0 120-30°, n20D 1.4711, d20 1.176, which was also obtained in the same manner from XVIII. III (11.8 g.) and 3.6 g. BzPh in 200 cc. CH2:CH0Et irradiated 88 hrs. at 20° and evaporated, and the residue chromatographed on silica gel gave 9 g. anhydride (XX) of 1,2-dimethyl-35ethoxycyclobutane-1,2-dicarboxylic acid (XXI), m. 62-4° (sublimed at 60°/0.3 mm.). XX (1.21 g.) in 100 cc. 1:1 H20-C6H6 refluxed several hrs. and evaporated gave 1.3 g. XXI, m. 200-3° (sublimed at 175°/0.3 ram.). XXI (0.93 g.) treated with CH2N2-Et2O, and the crude product chromatographed on silica gel yielded 0.99 g. di-Me ester of XXI, b0..3 110°, n20D 1.4493, d20 1.069. Coumarin (14.6 g.), 11.4 g. II, and 1.5 g. BzPh in 200 cc. C6H6 irradiated 23 hrs. at 15-20° and evaporated, and the residue boiled with Et20 left 6.4 g. 1,2-indeno-3,4-coumarinocyclobutane, m. 160.5° (sublimed at 100°/0.1 mm.). 14495-41-1P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Four-membered ring systems by photosensitized symmetrical and mixed cycloaddition)

14495-41-1 CAPLUS RN

1,2,3,4-Cvclobutanetetracarboxvlic acid, 1,2,3,4-tetramethvl ester (CA INDEX NAME)



CORPORATE SOURCE:

CN

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

L22 ANSWER 58 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN 1962:436298 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 57:36298

ORIGINAL REFERENCE NO.: 57:7239c-h

TITLE: Photosensitized cyclodimerization of coumarin

AUTHOR(S): Schenck, Guenther Otto; Wilucki, Iugeborg v.; Krauch, Carl Heinrich

Max-Planck-Inst. Kohleforsehung, Muehlheim, Germany

SOURCE: Chemische Berichte (1962), 95, 1409-12

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 57:36298 For diagram(s), see printed CA Issue.

Coumarin (I) without sensitization yielded II, with sensitization III and IV, upon irradiation. The 2 reactions do not have common intermediates. I (29 g.), m. 67-70°, and 5 g. BzPh, m. 48°, in 250 cc. C6H6 irradiated 60 hrs. at 10-15° gave 27.9 g. 111, m. 176.5° (EtOH, C6H6, AcOH and sublimed in vacuo); the mother liquor yielded 0.45 g. IV, m. 320-5° (sublimed); 4.57 g. BzPh was recovered. I (29 g.) in 250 cc. C6H6 irradiated 125 hrs. in glass or 45 hrs. in quartz gave

only unchanged I. I (12.3 g.) in 110 cc. absolute EtOH irradiated 46 hrs. gave 1.17 g. II, m. 260° (decomposition) (AcOH and sublimed in vacuo).

I (11.54 g.) and 3.08 g. BzPh in 150 cc. absolute EtOH irradiated 16 hrs. yielded 2.2 g. III. I (135 g.) irradiated 30 hrs. at 71-5° with an immersed quartz lamp gave 0.45 g. I. III (13 g.) in 700 cc. 80% AcOH ozonized 10 hrs. at 15° with about 25 g. 03/hr., treated with cooling with 250 co. 10% H2O2, kept 2 days, evaporated, the residue treated with Et2O-CH2N2, and chromatographed on silica gel yielded 70.8% tetra-Me cis-trans-cis-eyelobutanetetracarboxylate, m. 144.5°. III (3 g.) in 50 cc. 10% aqueous NaOH acidified with 10% HCl and filtered gave 3.5 q. dihydroxy-u-truxinic acid (V), m. 175° after melting with bubbling at 95° and resolidification at 150°. V refluxed 2 hrs. with Ac20 gave III. V (3.32 g.) and CH2N2-Et20 vielded 3.2 g. di-Me ester of V. m. 160° (decomposition). III (5 g.) with 9 g. Me2SO4 in 41 cc. 2N NaOH yielded 3.04 g. Me ester (VI) of dimethoxy-u-truxinic acid (VII), m. 137-8° (decomposition) (MeOH); the filtrate from the VI acidified with 10% HCl gave 3.07 g. VII, m. 200° (decomposition) (aqueous MeOH).

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 14495-41-1 CAPLUS
CN 1,2,3,4-Cyclobrusetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA

INDEX NAME)

IT 1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis,trans,cis-

RL: PREP (Preparation) (preparation of)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L22 ANSWER 59 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1962:429516 CAPLUS

DOCUMENT NUMBER: 57:29516 ORIGINAL REFERENCE NO.: 57:5853f-g

TITLE: Preparation of some 2,3:6,7-dibenzobiphenylenes

AUTHOR(S): Bruce, J. Malcolm CORPORATE SOURCE: Univ. Manchester, UK

SOURCE: Journal of the Chemical Society (1962) 2782-5

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB The photodimer (I) of 1,4-naphthoquinone was converted into

1,4,5,8-tetrahydroxy-2,3:6,7-dibenzobiphenylene, and the tetramethyl ether and tetraacetate of this compound were prepared Evidence is presented concerning structure of the enolic form of the obotodimer (II) of

2,3-dimethyl-1,4-benzoquinone.

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966)) RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

IT 1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis,trans,cis-

RL: PREP (Preparation)
(preparation of)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 60 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:429515 CAPLUS

DOCUMENT NUMBER: 57:29515

ORIGINAL REFERENCE NO.: 57:5853e-f

TITLE: Condensed cyclobutane aromatic compounds. XXI. Adducts of benzocyclobutadienes with 1,3-diphenylisobenzofuran AUTHOR(S): Cava, M. P.; Pohlke, R.

CORPORATE SOURCE: Ohio State Univ., Columbus, OH, USA

SOURCE: Journal of Organic Chemistry (1962), 27(5), 1564-7

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

AB Diphenylisobenzofuran has been found to be an excellent trapping agent for benzocyclobutadiene and for halogenated benzocyclobutadienes. Some chemical transformations of the adducts obtained are reported.

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L22 ANSWER 61 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:403716 CAPLUS

DOCUMENT NUMBER: 57:3716

ORIGINAL REFERENCE NO.: 57:6711,672a-e

TITLE: The chemistry of photodimers of maleic and fumaric

acids derivatives. III.

cis,trans,cis-1,2,3,4-Tetracyanocyclobutane; possible
precursors for tetramethylenecyclobutane

AUTHOR(S): Griffin, G. W.; Basinski, J. E.; Peterson, L. I.

CORPORATE SOURCE: Yale Univ.
SOURCE: Journal of the American Chemical Society (1962), 84,

1012-15

CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:3716

GI For diagram(s), see printed CA Issue.

AB The photodimerization of fumaronitrile (I) to

cis-trans,cis-tetracyanocyclobutane (II) in the solid state has been studied and the stereochem. of II correlated with the crystal lattice structure of I. The chemical of II has been investigated and a series of compds. derived from I have been synthesized. I deposited on the inside of a 1-1. graduated cylinder by evaporating a solution of I under N, the

deposit
irradiated 1 wk with a germicidal lamp and extracted with hot Et2O left 2.1 g.
II, p. 250° (decomposition) (MeCN). II (0.75 g.) added to 20 cc. AcOH

and 1 cc. concentrated HC1, heated to solution, concentrated, and filtered yielded 0.393

g. III, m. 325° (Me2CO); the filtrate treated with CH2N2-Et2O gave the tetra-CO2Me analog of II, m. 144-5°. II (8.0 g.), 150 cc.

Ac20, and 0.70 g. Pt02 hydrogenated 1 wk at about 25° yielded 4.0 g. tetra-AcNHCH2 analog (IV) of II, m. 278-9° (H2O). IV (6.0 g.)

g. tetra-AcNHCH2 analog (IV) of II, m. 278-9° (H2O). IV (6.0 g.) and 35 cc. concentrated HC1 heated 3 h. and evaporated, and the residue sublimed at

80°/0.5 mm. gave the extremely hygroscopic tetra-H2NCH2 analog (V) of II. V in 10% aqueous NaOH with BzCl yielded the tetra-BzNHCH2 analog of

II, m. 302-3° (hot EtOH). Tetraacid chloride (VI) of 1,2,3,4-cyclobutanecarboxylic acid, m. 76-7° (hexame), from the acid with PC15 in 200 cc. C6H6 treated 4 h. with stirring with gaseous Me2NH, heated to boiling, filtered, and evaporated gave 5.1 g. tetra-CONMe2 analog (VII) of II, m. 194-5° (Et20-C6H6). VII (5.1 g.) in 100 cc. Et20 and 100 cc. C6H6 refluxed through a Soxhlet thimble charged with 1.7 g. LialH4, refluxed 1 h., and worked up gave 3.1 g. Me2NCH2 analog (VIII) of II, b0.05 110-12°. MeI (4.0 g.) and 1.0 g. VIII in 50 cc. absolute MeOH refluxed overnight and cooled yielded 2.4 g. tetramethiodide of VIII. VIII (4.0 g.) added with stirring and cooling to 60% H2O2, warmed after 6 h. to room temperature, kept overnight, heated with a small amount of Pt-C, filtered, and treated with picric acid gave the picrate of the tetra-N-oxide of VIII, m. 219-20°. VI (3 g.) in 150 cc. C6H6 treated with gaseous NH3 gave some III.

(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 14495-41-1 CAPLUS
CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA

INDEX NAME)

TТ

IT 1032-95-7P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, cis,trans,cis-RI: PREP (Preparation)

(preparation of)

RN 1032-95-7 CAPLUS CN 1,2,3,4-Cvclobutane

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha,2\alpha,3\beta,4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 62 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1962:403715 CAPLUS

DOCUMENT NUMBER: 57:3715
ORIGINAL REFERENCE NO.: 57:670i,671a-i

TITLE:

The chemistry of photodimers of maleic and fumaric acids derivatives. II. The preparation of cis-trans.cis-and

trans, trans, trans-1,2,3,4-tetrabenzoylcyclobutane; the acid chlorides of 1,2,3,4-tetracarboxycyclobutanes

AUTHOR(S): Griffin, G. W.; Hager, R. B.; Veber, D. F. CORPORATE SOURCE: Yale Univ. SOURCE: Journal of the American Chemical Society (1962), 84, 1008-11 CODEN: JACSAT: ISSN: 0002-7863 DOCUMENT TYPE: Journal LANGUAGE: Unavailable cf. CA 55, 22159f. The acid chlorides of cis, trans, cis- (I) and trans, trans, trans-1, 2, 3, 4-tetracarboxycyclobutane (II) were prepared and employed as precursors for several sym. 1,2,3,4-tetrasubstituted cyclobutane derivs. Dry I from 22 g. tetra-Me ester (III) of I refluxed 3 h. with 63.2 g. PC15 and evaporated, the residue dissolved in 50 cc. dry C6H6, added dropwise with stirring to 40.4 g. AlCl3 in 300 cc. C6H6, stirred 2.5 h., poured into 500 cc. 10% HCl, stirred 1 h., and filtered, and the residue extracted 36 h. in a Soxhlet apparatus with 200 cc. CHCl3 gave 7.5 g. cis, trans, cis-1, 2, 3, 4-tetrabenzoylcyclobutane (IV), m. 259-61°. I (22.1 g.) and 79.2 g. PC15 refluxed 3 h. and distilled gave 17.5 g. tetraacid chloride (V) of I, m. 76-7° (repptd. from warm CC14 with hexane). V with MeOH gave III. II (20 g.) and 72.5 g. PC15 refluxed 5 h. gave 21.6 g. tetraacid chloride (VI) of II, b0.2 120-4°, m. 63-5°. VI with MeOH yielded 100% tetra-Me ester of II, m. 126-7°. VI (8.5 g.) in 120 cc. dry C6H6 added during 15 min. to 15.8 g. AlCl3 in 30 cc. C6H6 at 5°, stirred 6 h. with warming to 20°, and worked up, and the crude product extracted 24 h. with C6H6 in a Soxhlet apparatus gave 10 g. IV trans, trans, trans-isomer (VII), m. 254-6° (PhMe). V (0.5 g.) and 1 g. NaOMe in 60 cc. CHCl3 refluxed 15 min., diluted with H2O, and filtered, and the residue extracted with C6H6 in a Soxhlet apparatus gave 0.20 a. VII. IV heated 2.5 h. with 10% concentrated HCl in AcOH gave 13% VII. VII (1.0 g.) in 40 cc. dry THF added during 15 min. to PhMgBr from 2.7 g. PhBr and 0.48 g. Mg in 25 cc. dry THF, refluxed 1.5 h., and worked up, and the crude product extracted in a Soxhlet apparatus 0.5 h. with pentane, 0.5 h. with C6H6, and 12 h. with THF gave from the THF extract 0.25 g. trans, trans, trans-tetrakis (diphenylhydroxymethyl) cyclobutane, m. above 330°. VII (1.0 g.) extracted from a Soxhlet thimble into 0.15 g. LiAlH4 in THF during 8 h. gave 0.98 g. trans, trans, trans-tetrakis (a-hydroxybenzyl) cyclobutane (VIII), m. 256-8° (50% EtOH). VIII (1.0 g.), 1.0 g. Cu chromite, and 100 cc. EtOH hydrogenated 8 h. at 250°/2000 lb. initial pressure yielded 0.5 g. trans, trans, trans-tetrabenzylcylcobutane (IX), m. 123-4°, also obtained in the same manner directly from VII. IV (0.67 g.) and 15 cc. N2H4.H2O heated 15 h. on the steam bath and filtered and the residue sublimed at 200°/0.15 mm. gave 0.15 g. 3,6-diphenylpyridazine, m. 221-2.5° (Me2CO). CF3CO3H from 3.8 cc. (CF3CO)2O and 0.040 cc. 90% H202 in 6 cc. CH2C12 added during 15 min. with stirring to 3.6 g. NaH2P04 and 1.0 g. VII in 60 cc. CH2Cl2, refluxed 20 h., and poured into 300 cc. H2O, the organic layer worked up, the residue digested with C6H6 left 0.16 g. unchanged VII; the extract yielded 0.095 g. trans, trans, trans-tetracarbophenoxycyclobutane, m. 189-93° (C6H6).

VI (30 g.) in 100 cc. Bt20 added dropwise during 15 min. with stirring and cooling to 1.2 mol CH2N2 in 2 l. Et2O, stirred 1 h. at room temperature, and concentrated gave 30.2 g. diazo ketone; a 30.0-g. sample in 1 l. MeOH stirred 4 h. at 61° with 3.5 g. Ag2O and worked up, the crude product digested with 150 cc. boiling Bt2O, and the extract distilled yielded 9.8 g. tetra-Me ester (X) of trans,trans,trans-1,2,3,4-cyclobutanetetraacetic acid (XI), m. 59-61° (CCl4). X heated 0.5 h. at 60° in 20% H2SO4 and cooled gave 92% XI, needles, m. 310-12°. IX (1.0 g.) in 50 cc. 90% aqueous AcOH treated 8 h. at room temperature with 1.3 g. 03/h., kept 2

days at room temperature in 10 cc. 30% H2O2 in 26 cc. H2O, filtered, concentrated to $5\,$

cc., and kept overnight yielded 0.12 g. XI. VI (9.0 g.) in 125 cc. C6H6 treated with 7.6 g. activated NaN3, refluxed overnight, filtered hot, treated with 100 cc. concentrated HCl, refluxed 0.5 h. with stirring, and the aqueous layer concentrated to 25 cc. and filtered yielded 3.0 q. trans, trans, trans-1,2,3,4-tetraminocyclobutane-4HCl (XII.4HCl). XII.4HCl (0.050 g.) triturated with NaOH and heated at 100°/0.1 mm. gave an extremely hygroscopic sublimate which benzoylated by the Schotten-Baumann procedure yielded the tetrakis (N-Bz derivative) of XII, m. 308-10° (EtOH). Mg (1.05 g.) in 35 cc. dry THF treated with 3.24 g. iodine, the suspension treated with 50 cc. dry THF and 1.0 g. VII during 24 h. (added by extraction from a Soxhlet thimble) under N, hydrolyzed with 50 cc. H2O, kept 1 h., evaporated, acidified with dilute HCl, and extracted with C6H6 gave 0.03

g. (BzCH2)2, m. 143-4.5° (EtOH).

ΙT 14495-41-1 (Derived from data in the 7th Collective Formula Index (1962-1966))

14495-41-1 CAPLUS RN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA CN INDEX NAME)

OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD 1 (1 CITINGS)

L22 ANSWER 63 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:53033 CAPLUS

DOCUMENT NUMBER: 56:53033

ORIGINAL REFERENCE NO.: 56:9993i,9994a-i,9995a-b TITLE:

Organic sulfur compounds. IV. Some addition and cooxidation reactions of 4-chlorobenzenethiol with

dicyclopentadiene and Aldrin Oswald, Alexis A.; Noel, Fernand

AUTHOR(S): CORPORATE SOURCE: Imp. Oil Ltd., Sarnia, Can.

SOURCE: Journal of Organic Chemistry (1961), 26, 3948-57

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. CA 54, 21005e.-4-Chlorobenzenethiol (I) readily added to exo- (II) and endo-dicyclopentadienes (III) and Aldrin (IV) by a radical mechanism to yield the exo (V) and endo isomers of 4-chlorophenylthiodihydro-dicyclopentadiene (VI) and 2-(p-chlorophenylthio)-endo-5,6,7,8,9,9-hexachloro-exo-endo-1,2,3,4,4a,5,8,8a-octahydro-1,4,5,8-dimethanonaphthalene (VII). When I solns. were air oxidized with any of the above diolefins, unstable hydroperoxide intermediates, p-chlorophenylthiohydroperoxydihydro-endodicyclopentadiene (VIII), p-chlorophenylthiohydroperoxydihydro-exodicyclopentadiene (IX), and exo-2-(p-chlorophenylthio)-3-hydroperoxy-endo-5,6,7,8,9,9-hexachloro-exo-endo-1,2,3,4,4a,5,8,8a-octahydro-1,4:5,8dimethanonaphthalene (X) were obtained. The hydroperoxide intermediate of

the thiol-IX cooxidn., X, was isolated as a colorless crystalline substance. In solution, it rearranged to the corresponding 2-(p-chlorophenylsulfinyl)-3-hydroxy derivative (XI). It was suggested that

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were responsible for qum formation in some cracked gasolines. I was
     recrystd., m. 52-3° (heptane). Tech. IV was recrystd. from heptane
     then MeOH, m. 101-2°. III (13.2 g.) and 14.5 g. I mixed with rise
     in temperature, the temperature maintained below 70° by cooling, left 4 days at
     room temperature, and the mixture distilled gave 26.2 g. VI, b2 145-6°. III
     (13.2 g.) and 14.5 g. I each in 0.3 mole/1. concentration in heptane left 1
week
     under N, evaporated, and the residue distilled gave 25.5 g. VI. About 0.09 g.
     tert-butv1 hydroperoxide added to the heptane solution described above and
     left 1 week gave 93% VI. III (13.2 g.) and 29 g. I in heptane left 1 week
     gave 85% VI. Pure VI had n20D 1.6073. III (56 g.) and 224.5 g. aqueous HI
     stirred 12 hrs. under N with the temperature maintained below 50°,
     dissolved in Et20, washed, and distilled gave 116 g.
     iododihydro-exo-dicyclopentadiene (XII), b2 80-1°. XII (129.5 q.)
     and 67.2 g. KOH in 250 ml. 95% aqueous alc. refluxed 4 hrs. under N gave 40 g.
     II, b8 49-50°, n20D 1.5105. I (14.5 g.) and 13.2 g. II similarly
     treated gave 96% V, b2 146-7°, n20D 1.6053. VI 13.8 g.) in 40 ml.
     Ac20 and 15 ml. AcOH treated in 20 min. at about 50° with 11.2 q.
     30% H2O2, left 24 hrs. at room temperature, diluted with H2O, concentrated,
and the
     product crystallized gave 8.5 g. 4-chlorophenylsulfonyldihydro-endo-
     dicyclopentadiene (XIII), m. 113-14.5°. In another experiment, 14.5 g.
     I and 14.5 g. III gave the adduct and the crude adduct in 200 ml. AcOH
     oxidized by slowly adding 22.4 g. H202 at 40° gave 27.8 g. XIII.
     Similarly V gave 57% 4-chlorophenylsulfonyldihydro-exo-dicyclopentadiene
     (XIV), m. 84-5°. In another experiment, the oxidation of 27.7 g. V carried
     out in 200 ml. AcOH with 22.4 g. H202 gave 70% XIV. Heptane solns. of 2.9
     g. I and 7.3 g. IV were mixed under N and left I week at room temperature away
     from air to give 7.5 g. VII, m. 106.5-8.5°. A heptane solution (66
    ml.) of the reagents prepared as above was irradiated in a quartz flask by
     an ultraviolet lamp 1 hr. and the product crystallized to give 8.5 g. VII. VII
     (5.1 g.) in 40 ml. 1:1 AcOH-Ac2O treated at 40° with 0.34 g. H2O2
     in an aqueous 30% solution, the mixture kept 2 hrs. at that temperature, left
overnight
    at room temperature, concentrated, and the product crystallized gave two
isomeric
     sulfoxides, m. 206-8.5° and 190-3°, in 36% and 30% yields.
     VII (5.1 g.) oxidized with 0.68 g. H2O2 as 30% solution gave 4.5 g.
     exo-2-(p-chlorophenylsulfonyl)-endo-5,6,7,8,9,9-hexachloro-exo-endo-
     1, 2, 3, 4, 4a, 5, 8, 8a-octahydro-1, 4:5, 8-dimethanonaphthalene, m.
     223-6°. I (14.5 g.) in 320 ml. heptane treated with passage of
     air, 13.2 g. III added, the air introduction continued 2 hrs. at room
     temperature, and the product crystallized gave two hydroxyethylsulfoxide
isomers, m.
     218-20° and 182-4°. The heptane filtrate on evaporation left 7
     q. oil, which on vacuum distillation afforded 5 q. VI; oxidation gave
     p-chlorophenylsulfonyldihydro-endo-dicyclopentadiene. O introduced at
     -5° into a 160 ml. heptane solution of 3.6 g. I and 3.3 g. III, after
     1 hr. of oxygenation under ultraviolet light the liquor decanted, and
     cooled gave VIII, as crystals which became an oil at room temperature, n20D
     1.5820. From the heptane filtrate I q. crystalline solid was obtained, browned
    at 140^{\circ}, m. 175-85^{\circ}. The above peroxidic products were combined and recrystd. to yield 4.4 g.
     p-chlorophenylsulfinylhydroxydihydro-endo-dicyclopentadiene isomers
     described above. A 100 ml. heptane solution containing 4.8 g. I and 4.3 g. II
    aerated 2 hrs. and left overnight gave 4.1 g. semisolid. This was taken
     up in Me2CO, filtered, and the solid recrystd. to give 1.1 g.
    p-chlorophenylsulfinylhydroxydihydro-exo-dicyclopentadiene, m.
     167-8°. A 160 ml. heptane solution of 3.6 g. I and 3.3 g. II
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oxygenated at -5° under ultraviolet irradiation gave IX, unstable liquid, n200 1.5850. Into 333 ml. heptane solution containing 7.23 g. I and 18.25 g. IV air was introduced 3 hrs. at room temperature to give 9.7 g. X, m.

similar cooxidn. and not addition reactions of thiols and dicyclopentadiene

 $248-9\,^{\rm o}$ (decomposition). Another crystalline hydroxy sulfoxide isomer (XV) was obtained from the PhMe filtrate, m. $207-10\,^{\rm o}$. Also obtained

from the mother liquor was 0.5 g. VII. Into a 162 ml. pentane solution of 3.62 g. I and 9.12 g. IV air was introduced with irradiation with an

ultraviolet lamp to give after a total of $0.5~hr.~2~g.~XI.~On~heating~XI~m.~116-19°, solidified, m. <math>240-2^\circ.~Further~introduction~of$ air into the filtered mixture resulted in precipitation of a XI, X, and XV

mixture A

CC14 solution (15 ml.) of 0.27 g. XI left at room temperature gave 0.18 g. X.

CC14 solution (15 ml.) of 0.27 g. XI left at room temperature gave 0.18 g. X I 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L22 ANSWER 64 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1962:53032 CAPLUS

DOCUMENT NUMBER: 56:53032

ORIGINAL REFERENCE NO.: 56:99931

TITLE: Structure of Nenitzescu's dimer of benzocyclobutadiene

AUTHOR(S): Griffin, G. W.; Veber, D. F. CORPORATE SOURCE: Yale Univ.

SOURCE: Chemistry & Industry (London, United Kingdom) (1961)

1162

CODEN: CHINAG; ISSN: 0009-3068

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB cf. CA 54, 24612a.-Nenitzescu's hydrocarbon (I),

dibenzotricyclo[4.2.0.02,5]octa-3,7-diene, was ozonized. The product,

after esterification with diazomethane, was cis-trans-cis-1,2,3,4-tetracarbomethoxycyclobutane, yield 28%, m.

142-4° (MeOH). The two aromatic nuclei in I were trans.

IT 14495-41-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 14495-41-1 CAPLUS

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

1032-95-7P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (Structure of Nenitzescu's dimer of benzocyclobutadiene)

1032-95-7 CAPLUS RN

1,2,3,4-Cvclobutanetetracarboxvlic acid, tetramethvl ester, $(1\alpha, 2\alpha, 3\beta, 4\beta)$ - (CA INDEX NAME)

Relative stereochemistry.

L22 ANSWER 65 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1961:137115 CAPLUS DOCUMENT NUMBER: 55:137115

ORIGINAL REFERENCE NO.:

55:25787b-c TITLE:

Note on the all-cis-cyclobutane-1,2,3,4tetracarboxylic acid AUTHOR(S):

Criegee, Rudolf; Funke, Wolfgang CORPORATE SOURCE: Tech. Hochschule, Karlsruhe, Germany SOURCE: Chemische Berichte (1961), 94, 2358-9

CODEN: CHBEAM: ISSN: 0009-2940

Journal DOCUMENT TYPE:

LANGUAGE: Unavailable

Powdered peri-truxillic acid anhydride (1.0 g.) in 130 cc. AcOH treated 18 hrs. at room temperature with 1.65 g. ozone/hr. and then with 10 cc. 30% H2O2, the mixture kept 24 hrs., heated slowly to 80°, cooled, evaporated in vacuo at 35°, the residue dissolved in a min. of hot AcOH, and the solution diluted after cooling dropwise with petr. ether yielded 50% all-cis-cyclobutane-1,2,3,4-tetracarboxylic acid, platelets, decomposed from 200°; it gave with CH2N2 in tetrahydrofuran the tetra-Me ester, needles, m. 203-4° (after softening at 185°) (EtOAc and sublimed at 140°/0.01 mm.). The acid heated 1 hr. with Ac20 at

melting, rhombs from Ac20-dioxane. 14495-41-1P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetra-Me ester

100° gave the dianhydride, darkened above 235° without

RL: PREP (Preparation) (preparation of)

RN 14495-41-1 CAPLUS

ΙT

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

L22 ANSWER 66 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1961:118138 CAPLUS DOCUMENT NUMBER: 55:118138

ORIGINAL REFERENCE NO.: 55:22159f-i,22160a-c

TITLE: The chemistry of photodimers of maleic and fumaric acid derivatives. I. Dimethyl fumarate dimer AUTHOR(S): Griffin, G. W.; Vellturo, A. F.; Furukawa, K.

Yale Univ.

SOURCE: Journal of the American Chemical Society (1961), 83, 2725-8

CODEN: JACSAT: ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 55:118138

The irradiation of di-Me fumarate (I) in the solid state gave cis, trans, cis-1, 2, 3, 4-tetracarbomethoxycyclobutane (II), whose stereochemistry can be rationalized in terms of direct bond formation between nearest neighbor mols. in the crystal lattice of the monomer. The isomerization of II to the thermodynamically more stable trans, trans, trans-isomer (III) of II was readily achieved thermally. The reduction of III and the hydrolysis of II and III as well as their reactions with PhMgBr were also studied. I (10 g.) in Me2CO evaporated under N in a glass cylinder rotating in nearly horizontal position, an ultraviolet lamp inserted into the cylinder, the I irradiated 1-5 days at 25-30°, and the product extracted with C6H6 gave 60% II, m. 144-5°. II transesterified with PhCH2OH gave the tetra-PhCH2 ester, m. 107.5-8.5° (C6H6-hexane). II (1.0 g.) heated in a Pyrex tube at 0.1 mm. 20 hrs. at 300° gave 50% III, m. 123-5°. II (0.28 g.) refluxed 2 hrs. with 0.3 g. NaOMe in MeOH, diluted with 10 cc. 10% aqueous NH4Cl, evaporated, and sublimed at 80°/0.01 mm. gave 18% III, m. 127° (H2O). II (5 g.) heated with concentrated HCl to solution on a steam bath, and the resulting acid, which lost H2O at 220-5°, treated with CH2N2-Et2O gave II. III (0.28 g.) and 5 cc. concentrated HCl gave the tetra-CO2H analog of III, m. 261-4° (decomposition) [AcOH-hexane or tetrahydrofuran (THF)-hexane], which sublimed gave the chair dianhydride (IV). Tetra-CO2H analog (V) of II (0.10 g.) heated 3 hrs. with SOC12 and evaporated, and the residue washed with hexane and sublimed, gave IV. V heated at 225-30°/0.05 mm. gave also IV. IV was identical with the photodimerization product from maleic anhydride. IV (0.50 g.), 2.50 g. PbO2, and 10 g. powdered glass heated 0.25 hr. at 250° with stirring under a stream of N (CO2 was evolved) gave a residue containing no organic material. II (5.8 g.) in 150 cc. C6H6 and 150 cc. dry Et2O reduced with 3.0 g. LiAlH4 in the inverse manner and then treated dropwise with 25 cc. AcCl in 50 cc. Et20 and heated 12 hrs. gave 2.0 g. tetraacetate (VI) of cis, trans, cis-1,2,3,4-tetrakis(hydroxymethyl)cyclobutane (VII), b0.02 178-80°. VI (0.90 g.) and 2.0 g. KOH in 50 cc. MeOH refluxed 2 hrs. and evaporated, and the residue heated 3 hrs. with excess BzCl gave the tetrabenzoate of VII, m. 104-5°. V (1.0 g.) in 200 cc. boiling THF treated dropwise with 0.1 mole PhMgBr in 50 cc. dry THF gave 0.5 g. crystalline solid, m. 285-7° (decomposition) (C6H6); the infrared spectrum showed bands for a OH and a CO function. IV treated in 250 cc. THF dropwise with stirring with PhMgBr from 16 g. Mg, 72 cc. PhBr, and 75 cc. THF, the mixture refluxed 2 hrs., stirred 12 hrs. at room temperature, and worked up gave trans, trans, trans-1, 2, 3, 4-tetrakis (a-hydroxybenzhydryl) cyclobutane (VIII), m. above 300° (absolute EtOH). VIII (0.50 g.), 1.0 g. CuO-Cu-Ba-chromite catalyst, and 100 cc. EtOH hydrogenolyzed 8 hrs. at 250° and 1900 lb. initial H pressure yielded 0.25 g. trans, trans, trans-1, 2, 3, 4-tetrabenzhydrylcyclobutane, m. 284-7° (methylcyclohexane).

14495-41-1 103268-55-9

(Derived from data in the 6th Collective Formula Index (1957-1961)) RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

RN 103268-55-9 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetrakis(phenylmethyl) ester (CA INDEX NAME)

IT 1032-95-7P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (The chemistry of photodimers of maleic and fumaric acid derivatives.

Dimethyl fumarate dimer)

RN 1032-95-7 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, (1α,2α,3β,4β)- (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT:

6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L22 ANSWER 67 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1961:118137 CAPLUS

DOCUMENT NUMBER: 55:118137

ORIGINAL REFERENCE NO.: 55:22158e-i,22159a-f

TITLE: Dimethylketene dimer. I. Catalytic hydrogenation and ring cleavage by alcohols

AUTHOR(S): Hasek, Robert H.; Elam, Edward U.; Martin, James C.; Nations, Ronald G. CORPORATE SOURCE: Tennessee Eastman Co., Kingsport

Journal of Organic Chemistry (1961), 26, 700-4

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 55:118137

GI For diagram(s), see printed CA Issue.

AB Optimal conditions for hydrogenation of dimethylketene dimer (I) to the corresponding glycol (II) were sought and excellent yields obtained with a Ru-C catalyst. I (400 g.) in 600 ml. MeOH hydrogenated at 125°/1000-1500 lb./sg. in. 1 hr. with 20 g. 5% Ru-C with rocking in

a stainless steel autoclave and the filtered solution evaporated yielded 98%

II.

2,2,4,4-tetramethyl-1,3-cyclobutanediol, m. 129-50°. I (285 g.) in 400 ml. MeOH hydrogenated 18 hrs. at 150°/100 atmospheric with 20 g. Raney Ni, the filtered solution hydrogenated 5 hrs. with 50 g. Raney Ni under the same conditions, the filtered solution evaporated, the residue distilled in

vacuo,

the product (91 g., b2 50-80°) combined with material (140 g., b3 62-72°) from a similar run, and the mixture fractionated through an 8 ft. spinning band column (10:1 reflux ratio) gave 26 ml. Me2CHCOCMe2CO2R (III, R = Me) (IV), b3.1-3.4 51.0-1.8°, contaminated with a small amount of Me2CHCOCMe2CH2OH (V), and 25 ml. V, b3.5-3.6 62.6°, n20 D 1.4382, λ 2.9, 5.9, 7.3-7.4 μ; p-O2NC6H4CO derivative m. 83-4°. I (28 g.) in 300 ml. MeOH hydrogenated with 0.2 mole H with stirring at 40°/3 atmospheric with 4 g. Raney Ni in EtOH, the filtered solution evaporated, and the residue recrystd. from C6H6 yielded 70% 3-hydroxy-2,2,4,4-tetramethylcyclobutanone, m. 114°; 2,4-dinitrophenylhydrazone m. 154.5-6.0° (corrected). I (100 g.) and 100 g. MeOH autoclaved (N atmospheric) 12 hrs. at 160° and the filtered solution distilled yielded 32% IV, converted by N2H4 to 4,4-dimethyl-3-isopropyl-2-pyrazolin-5-one, m. 81.5-2.5° (corrected). Na (0.1 g.) in 100 ml. absolute alc. at 10° treated portionwise (external cooling) below 50° with 50 g. I, the mixture acidified with 2 ml. AcOH, and distilled yielded 87% III (R = Et). Me3COH (250 ml.)

containing 4 g. 50% dispersion of NaH in mineral oil stirred with 140 g. I, the mixture heated slowly to 60° to initiate an exothermic reaction, the

self-refluxing solution stirred 1 hr., acidified with 10 ml. AcOH, and

vielded 73% III (R = Me3C). I (70 q.), 15 q. HOCH2CH2OH, and 15 ml. C5H5N autoclaved 12 hrs. at 200° and the homogeneous product distilled gave 20 g. forerun and 77% III (R = CH2CH2) (bis compound). I (100 g.), 50 g. II, and 0.5 g. Na heated to 100°, the slurry treated with 2 ml. absolute alc. with immediate rise of temperature to 140-5°, the temperature maintained 45 min. before cooling, and the product repeatedly recrystd. from Me2CO vielded 57% III (R = HC.CMe2.CH.CMe2) (his compound), m. 113-14°. The base-catalyzed alcoholysis of I was used to prepare a series of esters. Further study showed that phenols and mercaptans were similarly esterified, although at a somewhat slower rate. I (80 g.), 53 g. PhOH, and 0.1 g. Na heated to 90°, 2 ml. absolute alc. added, heating continued to 190-5°, the mixture kept at this temperature 30 min., and the cooled mixture distilled yielded 86% III (R = Ph). I (70 g.) and 101 g. C12H25SH refluxed 3 hrs. with stirring with 0.5 g. Na in 300 ml. xylene, the low-boiling components removed at 215°/3 mm., and the residue distilled in a cyclic falling film mol. still at $78-88^{\circ}/0.02$ mm. gave 72% Me2CHCOCMe2COSR (VI, R = C12H25). Data for III and VI were tabulated [R, % yield, b.p./mm. or m.p. (solvent), and n20D given]. III: Me, 32, 88-91°/22, 1.4244; Et, 87, 81.5-82°/9.5, 1.4230; Me2CH, 54, 113-16°/36, 1.4209; H2C:CHCH2, 73, 95-6°/10, 1.4369; Bu, 18, 113-14°/14, 1.4288; Me3C, 73, 100-4°/16, 1.4212; Ph, 86, 95-6°/0.5, 1.4859; CH2CH2 (diester), 77, 185-7°/5.5, 1.4484; HOCH2CMe2CH2, 56, 130-9°/2.5-3.5,

1.4488; CH2CMe2CH2 (diester), 5, 184°/3.5, 1.4488; S(CH2CH2)2 (diester), 93.5, 110°/0.004, 1.4720; MeCH2C(CH2)3 (triester), 52, 140°/0.001, 1.4587; C(CH2)4 (tetraester), 57, 91-2° (Me2C0-C6H14; p-C6H4 (diester), 11, 106-7° (alc.), VI: C12H25, 72, 78-88°/0.02, 1.4705; CH2)6 (diester), 76, 108-33°/1.0, 1.4951; p-Me3CC6H4, 60, 58-9° (alc.). II (321 g.) and 276 g. HCO2H refluxed 5 hrs. in 200 ml. C6H6, the cooled solution refluxed 4 hrs. with 276 g. HCO2H, the cooled solution diluted with C6H6, the washed and dried solution evaporated, and the residue distilled through a 48 in. packed column yielded

g. 98%-pure 2,2,4,4-tetramethyl-1,3-cyclobutanediol diformate (VII), b53 132-3°. VII (315 g.) stored at 20° and filtered gave 167 g. solid, m. 58-65°, recrystd. from petr. ether to give 144 g. trans-II diformate (VIII), m. 67-8°. VIII (132 g.) in 900 ml. MeOH containing 2 g. Na kept 24 hrs. at 20°, treated with 9 ml. AcOH, evaporated on a steam bath, the residue taken up in 900 ml. boiling PhMe, the graduet at the property of the cooled mixture filtered gave 78 g.

oven-dried (108°) trans-II, m. 148°. The filtrate from VIII converted to the free glycol by methanolysis, the mixture of glycol isomers crystallized from PhMe to give 79 g. material, m. 130-54°, a sample (57 g.) refluxed in 400 ml. PhMe, the solution cooled to 80°, the supernatant liquid decanted, the crystalline residue taken up in 400 ml. boiling PhMe, cooled to 100°, the supernatant decanted, and the crystalline product (24 g., m. 160-3°) recrystal from 350 ml. PhMe yielded 22 g. pure cis-II, m. 162.5-3.5°. The configuration of the yielded 22 g. pure cis-II, m. 162.5-3.5°. The configuration of the spectra since cis-II contains 2 types of Me groups, whereas all Me groups in trans-III are equivalent. The dipole moments 2.39 and 2.10 D. for the cis and trans isomers were consistent with the previously described structural assignments.

IT 14495-41-1 103268-55-9

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 14495-41-1 CAPLUS CN 1,2,3,4-Cvclobutane

1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

RN 103268-55-9 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetrakis(phenylmethyl) ester (CA INDEX NAME)

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

L22 ANSWER 68 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1961:59429 CAPLUS

DOCUMENT NUMBER: 55:59429
ORIGINAL REFERENCE NO.: 55:11380b-d

TITLE: cis, cis, cis-1, 2, 3, 4-Tetracarbomethoxycyclobutane;

structure of β-heptacyclene

AUTHOR(S): Griffin, Garv W.; Veber, Daniel F.

CORPORATE SOURCE: Yale Univ.

SOURCE: Journal of the American Chemical Society (1960), 82,

6417

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. CA 54, 13019d. β-Heptacyclene I (cis, Ia) in 90% aqueous HOAc

ozonized $17~\rm hrs.$ at 25° with $3.66~\rm g.$ $03/\rm hr.,$ the reaction mixture kept $3~\rm days$ with $308~\rm H202$ at room temperature, the solvents evaporated, the residue

esterified with CH2N2 and recrystd. from xylene gave a 5.6% yield of cis,cis,cis-1,2,3,4-tetracarbomethoxycyclobutane (II), m. 203-5°,

 λ 3.34, 3.38, 5.72, 6.95, 8.34, 8.47, 9.31, 10.45, 12.00, 12.84

u. Similarly α-heptacyclene I (trans, III) gave

cis,trans,cis-1,2,3,4-tetracarbomethoxycyclobutane (IV). Both II and IV in a sealed tube 20 hrs. at 300 $^{\circ}$ could be isomerized to the

all-trans tetraester. The infrared spectrum of II was identical to a totally esterified but otherwise uncharacterized minor product obtained from the irradiation of maleic anhydride in cyclohexane by Criegee. II

was the last of the 4 possible tetracarbomethoxycyclobutanes to be synthesized.

31351-41-4P

RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation) (cis,cis,cis-1,2,3,4-Tetracarbomethoxycyclobutane; structure of B-heotacyclene)

RN 31351-41-4 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester, $(1\alpha, 2\alpha, 3\alpha, 4\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 14495-41-1, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester

(stereoisomers)

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L22 ANSWER 69 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1961:59428 CAPLUS DOCUMENT NUMBER: 55:59428

ORIGINAL REFERENCE NO.: 55:11379h-i,11380a-b

TITLE: The pyrolysis of fluorene

AUTHOR(S): Lang, Karl Friedrich; Buffleb, Herbert; Kalowy, Joseph CORPORATE SOURCE: Rutgerswerke Akt.-Ges., Castrop-Rauxel, Germany

SOURCE: Chemische Berichte (1961), 94, 523-6 CODEN: CHBEAM; ISSN: 0009-2940 DOCUMENT TYPE: Journal

DOCUMENT TYPE: LANGUAGE:

LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

37 For diagram(s), see printed or Issue.
AB The pyrolysis of fluorene (I) yielded 1,2:7,8-dibenzochrysene (II), a new hydrocarbon probably of the structure III, and rubicene (IV). I (4250 g.) pyrolyzed at 700-50° gave 3355 g. pyrolyzate which distilled gave

unreacted I and left 645 g. black-brown residue; the residue dissolved in dry xylene and chromatographed on Al2O3 gave 128 g. II, needles, m. 214-159, 48 g. III, needles, m. 288-9°, and 26 g. IV, red

needles, m. 304-5° (xylene); in one run a small amount of a

hydrocarbon, pale yellow needles, m. 437-45°, was also obtained; it was green in warm concentrated H2SO4. The ultraviolet absorption spectra of

III, and IV were recorded.

IT 14495-41-1, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester

(stereoisomers) RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 70 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1961:22472 CAPLUS

DOCUMENT NUMBER: 55:22472 ORIGINAL REFERENCE NO.: 55:4382c-i TITLE: Cyclobutane-1,2,3,4-tetracarboxylic acid
AUTHOR(S): Criegee, Rudolf; Hover, Hermann
CORPORATE SOURCE: Tech. Hochschule, Karlsruhe, Germany
SOURCE: Chemische Berichte (1960), 93, 2521-4

CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 55:22472
GI For diagram(s), see printed CA Issue.

AB The ozone degradation of truxillic acids (I) vielded 3 of the 4 possible cvclobutane-1,2,3,4-tetracarboxvlic acids (II). Powdered PhCH:CHCH:C(CO2H)2 (III) (100 g.) in 2 l. weakly acidic H2O stirred and irradiated 48 hrs. with an immersed ultraviolet lamp and filtered gave nearly 100% dimer (IV) of III, m. 195° (glacial AcOH). IV (100 g.) in 650 cc. glacial AcOH and 100 cc. H2O treated at -5 to 0° with 28-30 g. ozone (2.2-2.3 g./hr.) and then gradually with 750 cc. 10% H202 below 30° and kept 4-5 days gave 40-5 g. α -I, m. 274° (MeOH); in smaller runs the yield could be increased to about 75%. $\alpha-I$ (13.0 g.) in 600 cc. glacial AcOH and 100 cc. H2O treated 20 hrs. with 2.8 g. ozone/hr. then gradually with 270 cc. 10% H2O2 and evaporated after 2 days in vacuo below 40° gave 9.2 g. IVa, plates, m. about 240° with previous sintering (decomposition) (dioxane); tetra-Me ester (V), 90%, m. 145° (C6H6), from IIa with CH2N2 at 0°. IIa (4.0 g.) in 20 cc. Ac2O heated 0.5 hr. at 100-20°, cooled, and filtered yielded 2.52 g. dianhydride of IIa, turned brown above 300° without melting. γ -I (4.0 g.), m. 228° (aqueous EtOH), ozonized and treated with H2O2 in the usual manner yielded 80-90% IVb, m. 219° (precipitated from glacial AcOH with Et2O), also obtained similarly from epi-I; tetra-Me ester, rodlets, m. 73-4° (petr. ether), b0.15 134-7°. ε-I, m. 192°, yielded in the same manner 80-90% Va, m. 260-40 (decomposition) (precipitated from hot glacial AcOH with ligroine); tetra-Me ester m. 127° (C6H6-petr. ether). V (3.0 g.) reduced at 30-40° with 2 g. LiAlH4, the noncryst. product in C5H5N treated at 0° with excess p-MeC6H4SO2Cl, kept 24 hrs. at room temperature, and poured into H2O yielded 3.0 g. VI (R = OH), melted with decomposition (hot aqueous EtOH). VI (16 g.) and 14 g. NaI refluxed 4 hrs., filtered, evaporated, and the product isolated with CHC13 yielded 7.0 g. VI (R = I), m. 140° (EtOAc-MeOH).

IT 14495-41-1P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester RL: PREP (Preparation)

(preparation of) RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 71 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1961:22471 CAPLUS

DOCUMENT NUMBER: 55:22471 ORIGINAL REFERENCE NO.: 55:4381h-i,4382a-c

Cyclopropanes. VII. The absolute configuration of TITLE: trans-caronic and cis- and trans-umbellularic acids Walborsky, H. M.; Sugita, T.; Ohno, M.; Inouye, Y. AUTHOR(S):

CORPORATE SOURCE: Florida State Univ., Tallahassee

Journal of the American Chemical Society (1960), 82, SOURCE:

5255-6

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

For diagram(s), see printed CA Issue.

cf. CA 53, 16053a; 54, 15267a. Et diazoacetate (I) (0.042 mol) was added to 0.042 mol (-)-menthyl β , β -dimethylacrylate (II) at 130-40° and the mixture distilled to remove unreacted II, which was

treated once more with an equivalent amount of I to yield 65% crude adduct. The

adduct was saponified to yield 27% caronic acid (III), [a]20D

-5.05° (EtOH). The observed optical rotation corresponded to 15.9% asym. synthesis. To a xylene solution of dimethyldiazomethane was added 31.4 g. (-)-di-menthyl fumarate in xylene at 0-5° to yield 10.0 g. oil,

which was heated with 1.0 g. Cu powder at 160-70° until N evolution

ceased. The product distilled to yield 56% of adduct ester. Saponification vielded

25% trans-III, $[\alpha]$ 20D 2.0° (EtOH), 6.3% asym. synthesis. (5.0 g.) was added to 11.3 g. (-)-menthyl α-isopropylacrylate at

80° and maintained at that temperature until N evolution ceased. The addition product was saponified and the mixture of cis and trans acids

separated to

give 14.7% cis-umbellularic acid (IV), [α]16D -5.4° (CHCl3), 6% asym. synthesis. The trans-umbellularic acid (V) was isolated in 56.5%

yield, [α]16D -5.2° (acetone), 2.7% asym. synthesis. On the basis of the above asym. syntheses, the following absolute configurations were assigned to IV and V.

14495-41-1P, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester

RL: PREP (Preparation)

(preparation of) RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L22 ANSWER 72 OF 72 CAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 1960:67951 CAPLUS

DOCUMENT NUMBER: 54:67951 ORIGINAL REFERENCE NO.: 54:13019d-h

TITLE . Photodimerization of maleic and fumaric acid

derivatives

AUTHOR(S): CORPORATE SOURCE: SOURCE: Griffin, G. W.; Basinski, J. E.; Vellturo, A. F. Yale Univ.
Tetrahedron Letters (1960), (No. 3), 13-16

DOCUMENT TYPE:

Journal Unavailable

LANGUAGE: Unavailable

For diagram(s), see printed CA Issue. trans-(MeO2CCH:)2 (I), trans-(NCCH:)2 (II), and (OCCH:)20 (III) were AB irradiated in the solid state with formation of the corresponding cyclobutane derivs. The olefins were deposited in a thin layer on the inner surface of a glass tube by evaporation of a CHC13 or Et20 solution, the layer irradiated 7-10 days by an internally located Westinghouse 15 T 8 Germicidal Sterilamp (95% ultraviolet radiation in the 253.7 mu region), and the tube externally cooled with cold H2O. Irradiation of 10 g. I gave 2 g. 1,2,3,4-tetracarbomethoxycyclobutane (IV), m. 144-5°, λ 5.74, 5.80, 7.72, 8.33, 9.79, 10.55, 11.85, 12.21 μ (KBr), nuclear magnetic resonance spectrum peaks at τ 6.15, 6.20 (CDC13) in agreement with the structure assigned by Criegee. Treatment of (IV) with NaOMe in MeOH effected stereochem. equilibration and gave the all-trans ester, m. 127°. Irradiation of II 7 days and recrystn. of the Et20-insol. material from MeCN gave 1,2,3,4-tetracyanocyclobutane, m. 237-9° (decomposition), λ 4.43, 3.35, 7.98, 8.25, 8.72, 9.72, 9.54, 9.64, 10.47, 12.22 u, with the same stereo-chemistry as that of I (as shown by hydrolysis with HCl-AcOH and esterification with CH2N2 to give I). Irradiation of III and sublimation of the product (m. above 200°) at 93°/0.005 mm. to remove III and at

CODEN: TELEAY; ISSN: 0040-4039

1,2,3,4-cyclobutanetetracarboxylic acid, λ 5.40, 5.62 μ . 14495-41-1, 1,2,3,4-Cyclobutanetetracarboxylic acid, tetramethyl ester

200°/0.005 mm. gave a bisanhydride of

(stereoisomers)

RN 14495-41-1 CAPLUS

CN 1,2,3,4-Cyclobutanetetracarboxylic acid, 1,2,3,4-tetramethyl ester (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)